

ON EXISTENCE OF L^1 -SOLUTIONS FOR COUPLED BOLTZMANN TRANSPORT EQUATION AND RADIATION THERAPY TREATMENT OPTIMIZATION

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ABSTRACT. The paper considers a linear system of Boltzmann transport equations modelling the evolution of three species of particles, photons, electrons and positrons. The system is coupled because of the collision term (an integral operator). The model is intended especially for dose calculation (forward problem) in radiation therapy. We show under physically relevant assumptions that the system has a unique solution in appropriate (L^1 -based) spaces and that the solution is non-negative when the data (internal source and inflow boundary source) is non-negative. In order to be self-contained as much as is practically possible, many (basic) results and proofs have been reproduced in the paper. Existence, uniqueness and non-negativity of solutions for the related time-dependent coupled system are also proven. Moreover, we deal with inverse radiation treatment planning problem (inverse problem) as an optimal control problem both for external and internal therapy (in general L^p -spaces). Especially, in the case $p = 2$ variational equations for an optimal control related to an appropriate differentiable convex object function are verified. Its solution can be used as an initial point for an actual (global) optimization.

1. INTRODUCTION

The Boltzmann transport equation (BTE) is an integro-partial differential equation which physically is based on the conservation laws. It has applications in many fields of scientific computation, including in among others optical tomography, cosmic radiation, nanotechnology (e.g. plasma physics) and radiation therapy, which is considered in this paper. For general mathematical theory of BTE with relevant boundary conditions we refer to [5] and [19]. See also [11], [12], [20], [44] where the subject is considered from more physical point of view. For more recent issues related to BTE can be found [40], and some non-linear aspects in [7]. Finally, for topics related to Monte Carlo methods in the context of BTE, both from theoretical and practical points of view, we refer to [33] and [47].

From the computational point of view, the primary goal in radiation therapy is to generate dose distributions in such a way that the prescribed dose conforms as well as possible to the target volume, while healthy tissue, and especially the so-called critical organs, achieve as low dose as possible. One considers the desired dose distribution in the patient domain to be known. In *external radiotherapy* the problem is to find the optimal dose by defining the field intensity, that is the incoming particle flux, on (patches of) the patient surface, which can be regulated (controlled) by the relative position and orientation of the patient and the accelerator head, as well as by different mechanical devices therein such as jaws, wedges and multileaf collimators (MLCs). In *internal radiotherapy* the radioactive sources are to be positioned

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inside the patient tissue such that the desired dose distribution is achieved. The determination of the external particle flux (or the distribution of internal sources) required to deliver the desired dose distribution is called the *inverse treatment planning problem* (IRTP), which from mathematical point of view is an *inverse problem*. The calculation of particle fluxes or dose in the patient tissue when the incoming fluxes or internal sources are known, is called *dose calculation*, and it is considered as a *forward problem*.

The solution of IRTP always requires some *dose calculation model*. Classical examples of such models, and whose popularity is mainly explained by the limitations in computer technology until quite recently, are the so-called pencil beam calculation models (cf. [29], [39]). These models are based on the idea that the incident radiation beam is divided into beamlets (pencil beams) and the total dose is obtained as a superposition (e.g. by convolution) of doses contributed by these beamlets (pencil beam kernels), which themselves are calculated by a Monte Carlo simulation or other methods such as Fermi-Eyges theory, which is based on a rough approximation of BTE ([8], [39], [47]). Even though various kinds of corrections for pencil beam models have been proposed (see references mentioned in [34], for example), they remain inaccurate especially in regions which are highly non-homogeneous. On the other hand, one can develop various dose calculation models based on point (spread) kernels (see [39]) that result from a single interaction by an incident photon (for example) at a given point in homogeneous material. Like the pencil beam kernels above, the point kernels are typically calculated by Monte-Carlo simulations.

In radiation therapy BTE describes how radiation is scattered and absorbed in a tissue. The sources of high energy particles, such as photon or electrons may be on the surface of the patient (external therapy) or inside the patient close to the cancer tissue (internal therapy). In any case they mobilize three kinds of particles, photons, electrons and positrons, whose simultaneous evolution should be taken into account in the transport model. In this setting, the potential creation of (or contamination by) other heavy particles (such as neutrons) will not be taken into account since their contribution is negligible (cf. [47]) when the source beam consists of photons or electrons in the relevant range (say 6-15MeV) of energies.

Dose calculation models governed by the (linear) BTE are valid in inhomogeneous material. They take rigorously into account the scattering and absorption effects (phenomena emerging from particle/nuclear physics) in physically solid way. We assume here that the transport of radiation particles is ruled by the following linear coupled system of three BTEs (for a derivation of the linear BTE, see [4], [20], [5])

$$(1) \quad \omega \cdot \nabla \psi_j + \Sigma_j(x, \omega, E) \psi_j - K_j \psi = f_j(x, \omega, E), \quad j = 1, 2, 3$$

together with an inflow boundary condition

$$(2) \quad \psi_j|_{\Gamma_-} = g_j, \quad j = 1, 2, 3$$

where

$$K_j \psi = \sum_{k=1}^3 \int_S \int_I \sigma_{kj}(x, \omega', \omega, E', E) \psi_k(x, \omega', E') dE' d\omega', \quad j = 1, 2, 3.$$

The first term on the left in (1) is called a convection (or advection) operator, the second term is a scattering operator and the third one is a collision operator. On the right, the functions f_j represent the (internal) sources, and g_j in (2) are boundary sources. The system is *coupled* through the operators K_j (unless, of course, $\sigma_{jk} = 0$ for $j \neq k$). Here a solution $\psi = (\psi_1, \psi_2, \psi_3)$ of the problem (1)-(2) is a

vector-valued function whose components describe the particle number densities of photons, electrons and positrons, respectively. Its dynamical counterpart is given by (see section 6)

$$(3) \quad \frac{1}{\|v_j\|} \frac{\partial \psi_j}{\partial t} + \omega \cdot \nabla \psi_j + \Sigma_j(x, \omega, E) \psi_j - K_j \psi = f_j(x, \omega, E, t), \quad j = 1, 2, 3$$

where $\|v_j\|$ is the speed of the particle j , together with inflow boundary and initial condition

$$(4) \quad \psi_j|_{\Gamma_- \times [0, T]} = g_j,$$

$$(5) \quad \psi_j(0) = \psi_{0j}, \quad j = 1, 2, 3.$$

The dynamical solution is defined in seven-dimensional phase space (x, ω, E, t) ; position, angle (direction of velocity), energy of particles and time. In the steady state (stationary state) there is no time dependence, and so the phase space (x, ω, E) is six-dimensional. This is basically always the case in applications related to radiotherapy, because the relevant radiation field(s) ψ anyway reach the steady state nearly instantly ([10]).

In this paper we consider the existence of solutions for the above coupled system (1), (2) in spaces $L^p(G \times S \times I)^3$ especially for $p = 1$. Here $G \subset \mathbb{R}^3$ is the spatial domain, $S \subset \mathbb{R}^3$ is the unit sphere and $I = [E_0, E_m]$ is the energy interval. The energy E and the angle ω are kept everywhere separated that is, the phase space is $G \times S \times I$. At first we consider the so-called escape time mapping $t = t(x, \omega)$ and recall of its analytical properties, which are useful e.g. in investigations of regularity of the solutions. After that we reproduce the well-known solutions (modified to our situation) of the convection/scattering equation (i.e. without the collision operator), by using the Lagrange's method i.e. the method of characteristics. Then the m -dissipativity property of the convection operator under homogeneous inflow boundary data is shown for one type of particles (again modified to our case). It follows from these considerations that the convection operator (under homogeneous inflow boundary data) is m -dissipative in the spaces $L^1(G \times S \times I)^3$ related to system (1), which is still uncoupled (section 5.1). Under certain, physically relevant assumptions we show the dissipativity of the (coupled) scattering-collision operator. Putting these together and applying the properties of m -dissipative operators and the lifting results of inflow boundary data, the existence and uniqueness result of solutions for coupled system (1), (2) is proved. In addition, we verify non-negativity of solutions when the data is non-negative. In section 6 the existence of solutions of the time-dependent coupled system (3), (4), (5) is studied.

The above model of transport is linear and, therefore, neglects any non-linear interaction (cf. [20], [24]). In addition the inflow boundary condition (2) is not exactly correct because minor part of the particles return to the patient domain G . The reflection boundary conditions of the form $\psi_j|_{\Gamma_-} = R_j(\psi_j|_{\Gamma_+}) + g_j$, $j = 1, 2, 3$, where R_j are appropriate (unbounded) operators might be more accurate (see [19], [36]).

The use of BTE in dose calculation needs the choice of *total and differential cross-sections*. In radiation therapy the cross-sections of primary interest are those for water (tissue), bone and air (void-like regions). For a more thorough discussion on the cross sections relevant to radiation therapy, we refer to [9], [31].

The analytical (explicit) solution of BTE is known only when the underlying geometrical settings, the structures of cross-sections, the sources and the incoming fluxes of particles (boundary conditions) are rather simple (see e.g. [20], Ch. 2).

Hence in practical situations one must apply appropriate numerical schemes for obtaining the solutions. Various kinds of numerical methods can be utilized for solving the transport equation (see [1]), for instance the combination of finite element method (or collocation method) and discrete ordinate method, or Monte Carlo.

In dose calculation the electron (and positron) transport is *forward-peaked* which implies additional challenges for computation. To diminish computational complexity, one possibility is to apply the so-called *continuous slowing down approximation* (CSDA) for the electron (and positron) evolution. CSDA means the use of the following equation (cf. [23], [34])

$$(6) \quad -\frac{\partial(S_{j,r}\psi_j)}{\partial E} + \omega \cdot \nabla \psi_j + \Sigma_{j,r}(x, \omega, E)\psi_j - K_{j,r}\psi = f_j(x, \omega, E), \quad j = 2, 3$$

instead of (1) for $j = 2, 3$ (electrons and positrons) where

$$\begin{aligned} K_{2,r}\psi &= \int_S \int_I \sigma_{1,2}(x, \omega', \omega, E', E)\psi_1(x, E', \omega')dE'd\omega' \\ &\quad + \int_S \int_I \sigma_{2,2,r}(x, \omega', \omega, E', E)\psi_2(x, E', \omega')dE'd\omega' \\ &\quad + \int_S \int_I \sigma_{3,2}(x, \omega', \omega, E', E)\psi_3(x, E', \omega')dE'd\omega' \end{aligned}$$

and

$$\begin{aligned} K_{3,r}\psi &= \int_S \int_I \sigma_{1,3}(x, \omega', \omega, E', E)\psi_1(x, E', \omega')dE'd\omega' \\ &\quad + \int_S \int_I \sigma_{2,3}(x, \omega', \omega, E', E)\psi_3(x, E', \omega')dE'd\omega' \\ &\quad + \int_S \int_I \sigma_{3,3,r}(x, \omega', \omega, E', E)\psi_3(x, E', \omega')dE'd\omega'. \end{aligned}$$

Above, for $j = 2, 3$, functions $\Sigma_{j,r}(x, E)$ are the *restricted total cross-sections*, $\sigma_{j,j,r}(x, E', E, \omega', \omega)$ are the *restricted differential cross-sections*, and the factors $S_{j,r} = S_{j,r}(x, E)$ are the so-called *restricted stopping powers*. The model neglects soft inelastic interactions. Besides the inflow boundary condition (2), one must demand from this model that the solution satisfy

$$\psi_2(x, \omega, E_m) = \psi_3(x, \omega, E_m) = 0,$$

or at least that

$$\lim_{E \rightarrow \infty} \psi_2(x, \omega, E) = \lim_{E \rightarrow \infty} \psi_3(x, \omega, E) = 0,$$

where in the last case we naturally assume that $I = [E_0, \infty[$. This requirement makes the overall problem mathematically well-defined that is, under relevant physical assumptions the problem has an unique solution. Similarly we can replace the equation (3) for $j = 2, 3$ in the time-dependent case to obtain a time-dependent CSDA. For stationary single CSDA equation existence of solutions and some optimal control results in L^2 -spaces are recently shown in [23] assuming that the stopping power is independent of the spatial coordinate x and that the collision operator has a special form. We will leave the considerations of the CSDA of BTE to a future work.

In section 7 we consider the above mentioned IRTP problem. In solving the IRTP problem one may use physical or biological criteria for optimization (for some general backgrounds see e.g. [48]). We consider here only physical criteria which are common in practical planning. Biological criteria are not considered, because their

grounds from the modelling perspective have not been well established. We notice, however that the optimization schemes given in this paper can also be founded on the biological criteria in an analogous manner, although the resulting object function is likely to be more multiextremal.

The patient domain $G \subset \mathbb{R}^3$ consists of tumor volume \mathbf{T} , critical organ's region \mathbf{C} and the normal tissue's region \mathbf{N} . Hence $G = \mathbf{T} \cup \mathbf{C} \cup \mathbf{N}$ where the union is mutually disjoint. The tumor volume (that is, the target) includes the tumor and some safety margin. Critical organs and normal tissue are build up of healthy tissue, and should receive as low a dose as possible.

Typically the resulting object function based on the physical criteria is, in the stationary case, of the form (see section 7.2)

$$(7) \quad \begin{aligned} J(f, g) = & c_{\mathbf{T}} \|D_0 - \mathcal{D}(f, g)\|_{L^p(\mathbf{T})}^p + c_{\mathbf{C}} \|(D_{\mathbf{C}} - \mathcal{D}(f, g))_-\|_{L^p(\mathbf{C})}^p \\ & + c_{\mathbf{N}} \|(D_{\mathbf{N}} - \mathcal{D}(f, g))_-\|_{L^p(\mathbf{N})}^p \\ & + c_{\text{DV}} \left(\left(v_{\mathbf{C}} - \frac{1}{\mathcal{L}^3(\mathbf{C})} \int_{\mathbf{C}} H((\mathcal{D}(f, g))(x) - d_{\mathbf{C}}) dx \right)_- \right)^p \end{aligned}$$

and where $c_{\mathbf{T}}, c_{\mathbf{C}}, c_{\mathbf{N}}, c_{\text{DV}}$ are positive weights, \mathcal{L}^3 is the 3-dimensional Lebesgue measure, H is the Heaviside function and a_- denotes the negative part of $a \in \mathbb{R}$. Here $\mathcal{D}(f, g) = D(\psi(f, g))$ where D is the dose operator (see section 7.2.1) and $\psi = \psi(f, g)$ is the solution of (1)-(2). We note that $f = 0$ for external therapy and $g = 0$ for internal therapy. In (7) the first three terms are convex and (locally) Lipschitz continuous (for $p = 2$ the first term is also differentiable), and the last term is both non-convex and non-differentiable in general. Moreover, the last term can be replaced a by Lipschitz continuous counterpart by replacing Heaviside function H with its definition by a Lipschitz continuous approximation (which in practice is reasonable). After this replacement the whole object function (7) is (locally) Lipschitz continuous. In addition the admissible sets (as given in section 7.2) are convex.

In practice, solving deterministically (i.e. without Monte Carlo methods) the discretized BTE is a quite formidable numerical task because in three spatial dimensions we have in total $3+2+1 = 6$ phase space variables (i.e. 3 spatial, 2 angular and 1 energy dimensions). In time-dependent case one would also have to take the time variable t into account, further increasing the state space dimension by one. We also notice that the collision term of BTE necessitates, in general, the consideration of two additional variables ω', E' which, however, are not phase space variables *per se*. Hence the numerical dimension of the problem is very large in the sense that the total number of grid points needed in any (deterministic) discretization scheme grows fast (to 6th or 7th power, say) with the number of grid points used for discretizing each individual dimension (if assumed to be proportional). There have only been a few attempts to solve BTE using deterministic methods for radiotherapy needs in three spatial dimensions without further approximations and/or geometrical simplifications (see e.g. [9]). In [31] computationally less complex algorithm is developed and some simulations are carried out in slab 3D-geometry.

Since the object function (7) contains nonconvex terms, *global optimization* for (locally) Lipschitz continuous functions in convex domains is needed. Moreover, the applied optimization method should be reasonably fast. Hence a careful initialization (determination of initial solution for optimization scheme) is necessary. We prove in section 7.2 (in the case $p = 2$) that for a certain related (convex) object function, the optimal control exists, and formulas for it in a variational form are given. We

suggest that this solution is used as an initial solution. Preliminary simulations show that the computation of the initial solution in this way is fast enough ([9]). In section 7 we bring up some challenges and problems related to IRTP.

Finally, we remark that an optimization scheme can be formulated in such a way that in external therapy the device (such as MLC) parameters are *directly* as decision parameters both in static and dynamical delivery techniques. This is based on the fact that the incoming flux g can be expressed as a function of these parameters, say $g = g(\mathbf{q})$ (see [50] for a certain implementation related to MLC). Substitution of this expression $g = g(\mathbf{q})$ to $\mathcal{D}(0, g)$ gives the object function (7) as a function of \mathbf{q} . The resulting object function is, however, highly multiextremal, and thus seeking its global minimum is rendered more difficult.

The authors would, moreover, like to mention that in [50], p.121 one must add for functions in H the requirement $f|_{\Gamma} \in L_2(\Gamma, |\omega \cdot \nu| d\sigma dE d\Omega)$ which is erroneously omitted there. In addition, in [51], p. 824 the space H should be the completion of $C^1(\bar{V} \times I \times S)$ with respect to $\langle \cdot, \cdot \rangle_H$ -inner product; not only the intersection $H_1 \cap H_2$ as it was erroneously defined there.

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2. NOTATIONS AND GENERAL ASSUMPTIONS

We assume that G is an open bounded set in \mathbb{R}^3 (equipped with Lebesgue measure) with piecewise smooth (orientable) C^1 boundary ∂G , that is, ∂G is 2-dimensional (orientable) piecewise C^1 -manifold (i.e. a C^1 -manifold with corners) such that G lies locally only on one side of ∂G , see e.g. [26], [35]. For example, G may be a parallelepiped.

The unit outward pointing normal on ∂G is denoted by ν and the surface measure on ∂G is $d\sigma$. Let S be the unit sphere in \mathbb{R}^3 equipped with the usual surface measure $d\omega$ and let I be the (energy) interval $[E_0, E_m]$, $E_0 \geq 0$ (which we assume to be bounded). The variable in S (in I) is denoted by ω (by E).

Let $(\partial G)_r$ be the C^1 -part of ∂G . We use the following abbreviations

$$\begin{aligned} \Gamma &= \{(y, \omega, E) \in \partial G \times S \times I\} \\ \tilde{\Gamma} &= \{(y, \omega, E) \in (\partial G)_r \times S \times I\} \\ \Gamma_+ &= \{(y, \omega, E) \in (\partial G)_r \times S \times I \mid \omega \cdot \nu(y) > 0\} \\ \Gamma_- &= \{(y, \omega, E) \in (\partial G)_r \times S \times I \mid \omega \cdot \nu(y) < 0\} \\ \tilde{\Gamma}_0 &= \{(y, \omega, E) \in (\partial G)_r \times S \times I \mid \omega \cdot \nu(y) = 0\}. \\ \Gamma_0 &= \tilde{\Gamma}_0 \cup (\Gamma \setminus \tilde{\Gamma}). \end{aligned}$$

Then $\Gamma = \Gamma_+ \cup \Gamma_- \cup \Gamma_0 \cup (\Gamma \setminus \tilde{\Gamma})$ and the union is mutually disjoint. Notice that Γ_{\pm} are open sets in $\partial G \times S \times I$ and $\Gamma \setminus \tilde{\Gamma} = (\partial G \setminus (\partial G)_r) \times S \times I$ is zero-measurable in Γ . Moreover, Γ_0 is a closed set in Γ , and it is in fact zero measurable as demonstrated in the following lemma.

Lemma 2.1 The set Γ_0 is zero-measurable in Γ .

Proof. It is enough to show that $\tilde{\Gamma}_0$ is zero-measurable in $\tilde{\Gamma}$. For each $y \in (\partial G)_r$ the set

$$S_0(y, E) = \{\omega \in S \mid \omega \cdot \nu(y) = 0\}$$

is zero-measurable in S (w.r.t the measure $d\omega$) and $\tilde{\Gamma}_0$ can be written as

$$\tilde{\Gamma}_0 = \{(y, \omega, E) \in \partial G \times S \times I \mid (y, E) \in (\partial G)_r \times I, \omega \in S_0(y, E)\}$$

Hence by Fubini's theorem (with dE is the Lebesgue measure on I , again with a slight abuse of notation)

$$(d\sigma \otimes d\omega \otimes dE)(\tilde{\Gamma}_0) = \int_{(\partial G)_r \times I} \left(\int_{S_0(y)} d\omega \right) d\sigma(y) dE = 0.$$

This finished the proof. \square

Remark 2.2 If ∂G happened to be piecewise C^2 -manifold, the proof of the zero-measurability of $\tilde{\Gamma}_0$ in $\tilde{\Gamma}$ above could also be proved in the following way that is more differential geometric in flavor:

Let $f : \tilde{\Gamma} \rightarrow \mathbb{R}$; $f(y, \omega, E) = \omega \cdot \nu(y)$, which is C^1 -smooth and $\tilde{\Gamma}_0 = f^{-1}(0)$. The differential Df of f on $\tilde{\Gamma}$ can be seen to be

$$Df(y, \omega, E)(a, b, c) = (D\nu(y)a) \cdot \omega + \nu(y) \cdot b, \quad (a, b, c) \in T_y(\partial G)_r \times T_\omega S \times \mathbb{R}.$$

Clearly, if $f(y, \omega, E) = 0$, then $Df(y, \omega, E) \neq 0$. Indeed, otherwise, as $\nu(y) \cdot b = 0$ for all $b \in T_\omega S$, there would be an $\alpha \in \mathbb{R}$ such that $\nu(y) = \alpha\omega$, hence $0 = f(y, \omega, E) = \alpha \|\omega\|_{\mathbb{R}^3}^2 = \alpha$, which is impossible as this would imply that $\nu(y) = 0$. Then $\tilde{\Gamma}_0$ is a C^1 -submanifold of $\tilde{\Gamma} = (\partial G)_r \times S \times I$ of codimension 1, and so has measure zero.

Furthermore, let

$$W^1(G \times S \times I) = \{\psi \in L^1(G \times S \times I) \mid \omega \cdot \nabla \psi \in L^1(G \times S \times I)\}$$

(here ∇ is taken with respect to x -variable only and $\nabla \psi$ is understood in the distributional sense). The space $W^1(G \times S \times I)$ is equipped with the norm

$$\|\psi\|_{W^1(G \times S \times I)} = \|\psi\|_{L^1(G \times S \times I)} + \|\omega \cdot \nabla \psi\|_{L^1(G \times S \times I)}.$$

Then $W^1(G \times S \times I)$ is a Banach space. It is known that the space

$$\mathcal{D}(\overline{G} \times S \times I) = \{\phi|_{G \times S \times I} \mid \phi \in C_0^\infty(\mathbb{R}^3 \times S \times \mathbb{R})\}$$

is dense in $W^1(G \times S \times I)$ (cf. [19], p. 221 and the references mentioned therein).

For Γ_- we use can define the space of L^1 -functions with respect to the measure $|\omega \cdot \nu| d\sigma d\omega dE = -\omega \cdot \nu d\sigma d\omega dE$ which is denoted by $T^1(\Gamma_-)$ that is, $T^1(\Gamma_-) = L^1(\Gamma_-, |\omega \cdot \nu| d\sigma d\omega dE)$. The norm in $T^1(\Gamma_-)$ is

$$\|h\|_{T^1(\Gamma_-)} = \int_{\Gamma_-} |h(y, \omega, E)| |\omega \cdot \nu| d\sigma d\omega dE.$$

The space $T^1(\Gamma_+)$ of L^1 -functions (and its norm) on Γ_+ with respect to the measure $|\omega \cdot \nu| d\sigma d\omega dE = \omega \cdot \nu d\sigma d\omega dE$ is defined similarly. Moreover, one has the following trace theorem (see [19], pp. 230-231).

Theorem 2.3 For any compact set $K \subset \Gamma_\pm$ there exists a constant $C_K > 0$ such that

$$\int_K |\psi(y, \omega, E)| |\omega \cdot \nu| d\sigma d\omega dE \leq C_K \|\psi\|_{W^1(G \times S \times I)} \text{ for all } \psi \in \mathcal{D}(\overline{G} \times S \times I).$$

Proof. We assume here, for definiteness, that $K \subset \Gamma_+$, the case $K \subset \Gamma_-$ being proven in analogous way. For $(\omega, E) \in S \times I$, let $K_{(\omega, E)} = \{x \in \mathbb{R}^3 \mid (x, \omega, E) \in K\}$ which is a compact subset of ∂G . Choose a function $\theta_K \in \mathcal{D}(\mathbb{R}^3 \times S \times \mathbb{R})$ such that $0 \leq \theta_K \leq 1$ everywhere, $\theta_K|_K = 1$ and $(\text{supp } \theta_K) \cap \Gamma_- = \emptyset$. Then as $\theta_K(x, \omega, E)(\omega \cdot \nu(x)) \geq 0$ for all $x \in (\partial G)_r$ and $\theta_K(x, \omega, E) = 1$ for all $x \in K_{(\omega, E)}$, and because $|\psi(\cdot, \omega, E)|$ belongs to the standard Sobolev space of index $(1, 1)$ on G i.e. to $W^{1,1}(G) = \{f \in L^1(G) \mid \nabla f \in L^1(G)\}$, we have

$$\begin{aligned} \int_{K_{(\omega, E)}} |\psi(\cdot, \omega, E)|(\omega \cdot \nu) d\sigma &= \int_{K_{(\omega, E)}} |\psi(\cdot, \omega, E)| \theta_K(\cdot, \omega, E)(\omega \cdot \nu) d\sigma \\ &\leq \int_{\partial G} |\psi(\cdot, \omega, E)| \theta_K(\cdot, \omega, E)(\omega \cdot \nu) d\sigma = \left| \int_G \omega \cdot \nabla (\theta_K(\cdot, \omega, E) |\psi(\cdot, \omega, E)|) dx \right| \\ &\leq \int_G |\omega \cdot \nabla \theta_K(\cdot, \omega, E)| |\psi(\cdot, \omega, E)| dx + \int_G |\theta_K(\cdot, \omega, E)| |\omega \cdot \nabla |\psi(\cdot, \omega, E)|| dx, \end{aligned}$$

where in the third phase we used the Stokes' Theorem, along with the fact that the integral over ∂G on the left is non-negative. Letting $C_K > 0$ be such that $|\theta_K| \leq C_K$ and $\|\nabla \theta_K\|_{\mathbb{R}^3} \leq C_K$ on $\mathbb{R}^3 \times S \times \mathbb{R}$, taking into account that $\nabla |\psi(\cdot, \omega, E)| = \text{sgn}(\psi(\cdot, \omega, E)) \nabla \psi(\cdot, \omega, E)$ (cf. [27], Section 5.1) we have, by integrating the above inequalities over $S \times I$,

$$0 \leq \int_K |\psi(x, \omega, E)|(\omega \cdot \nu) d\sigma(x) d\omega dE \leq C_K (\|\psi\|_{L^1(G \times S \times I)} + \|\omega \cdot \nabla \psi\|_{L^1(G \times S \times I)}).$$

The right hand side being equal to $C_K \|\psi\|_{W^1(G \times S \times I)}$, this finishes the proof. \square

Remark 2.4 Since $|\omega \cdot \nu|$ is bounded from below on a compact $K \subset \Gamma_-$, the previous inequality implies

$$\int_K |\psi(y, \omega, E)| d\sigma d\omega dE \leq \tilde{C}_K \|\psi\|_{W^1(G \times S \times I)},$$

for some constant $\tilde{C}_K > 0$ depending on K .

As a direct consequence of Theorem 2.3, any element $\psi \in W^1(G \times S \times I)$ has a well defined trace $\psi|_{\Gamma_-}$ in $L^1_{\text{loc}}(\Gamma_-, |\omega \cdot \nu| d\sigma d\omega dE)$ defined by

$$\psi|_K := \lim_{j \rightarrow \infty} \phi_j|_K \text{ for any compact subset } K \subset \Gamma_+,$$

where $\{\phi_j\} \subset \mathcal{D}(\overline{G} \times S \times I)$ is any sequence such that $\lim_{j \rightarrow \infty} \|\phi_j - \psi\|_{W^1(G \times S \times I)} = 0$. In addition the trace mapping $\gamma_- : W^1(G \times S \times I) \rightarrow L^1_{\text{loc}}(\Gamma_-, |\omega \cdot \nu| d\sigma d\omega dE)$; $\gamma_-(\psi) = \psi|_{\Gamma_-}$ is continuous.

In a similar way one has a continuous trace mapping $\gamma_+ : W^1(G \times S \times I) \rightarrow L^1_{\text{loc}}(\Gamma_+, |\omega \cdot \nu| d\sigma d\omega dE)$. Hence we can define (a.e. unique) the trace $\gamma(\psi)$ on Γ for $\psi \in W^1(G \times S \times I)$ by setting (recall that Γ_0 has a measure zero)

$$\gamma(\psi)(y, \omega, E) = \begin{cases} \gamma_+(\psi)(y, \omega, E), & (y, \omega, E) \in \Gamma_+ \\ \gamma_-(\psi)(y, \omega, E), & (y, \omega, E) \in \Gamma_- \\ 0, & (y, \omega, E) \in \Gamma_0 \end{cases}.$$

Finally we denote by $T^1(\Gamma)$ the space of L^1 -functions on Γ with respect to the measure $|\omega \cdot \nu| d\sigma d\omega dE$ that is,

$$T^1(\Gamma) = L^1(\Gamma, |\omega \cdot \nu| d\sigma d\omega dE).$$

The norm in $T^1(\Gamma)$ is

$$\|h\|_{T^1(\Gamma)} = \int_{\Gamma} |h(y, \omega, E)| |\omega \cdot \nu| d\sigma d\omega dE.$$

Evidently, the spaces $T^1(\Gamma_-)$ and $T^1(\Gamma_+)$ are isometrically embedded into $T^1(\Gamma)$ through the operation of extension by zero. From the fact that Γ_0 has a measure zero in Γ it follows that one can isometrically identify $T^1(\Gamma)$ with $T^1(\Gamma_-) \times T^1(\Gamma_+)$ (as can be seen easily). One can, moreover, identify the spaces $T^1(\Gamma_-)$ and $T^1(\Gamma_+)$ with each other isometrically, a result whose justification will be postponed until Corollary 5.9 (alternatively, see [16], Corollary 2.2 or [14]). As a consequence of these remarks, the space $T^1(\Gamma)$ can be identified isomorphically (i.e. with equivalent norm) with $T^1(\Gamma_-)$, or with $T^1(\Gamma_+)$.

The trace $\gamma_{\pm}(\psi)$ for $\psi \in W^1(G \times S \times I)$ is not necessarily in the space $T^1(\Gamma)$. Hence it is reasonable to define the space

$$\tilde{W}^1(G \times S \times I) = \{\psi \in W^1(G \times S \times I) \mid \gamma(\psi) \in T^1(\Gamma)\}.$$

The space $\tilde{W}^1(G \times S \times I)$ is equipped with the norm

$$\|\psi\|_{\tilde{W}^1(G \times S \times I)} = \|\psi\|_{W^1(G \times S \times I)} + \|\gamma(\psi)\|_{T^1(\Gamma)}.$$

As the spaces $T^1(\Gamma)$, $T^1(\Gamma_-)$ and $T^1(\Gamma_+)$ are mutually isomorphic, so are also the spaces $\tilde{W}^1(G \times S \times I)$, $\tilde{W}_-^1(G \times S \times I)$ and $\tilde{W}_+^1(G \times S \times I)$, where

$$\tilde{W}_{\pm}^1(G \times S \times I) := \{\psi \in W^1(G \times S \times I) \mid \gamma_{\pm}(\psi) \in T^1(\Gamma_{\pm})\},$$

equipped with the norms defined similarly as $\|\cdot\|_{\tilde{W}^1(G \times S \times I)}$ above.

Proposition 2.5 The spaces $\tilde{W}^1(G \times S \times I)$ and $\tilde{W}_{\pm}^1(G \times S \times I)$ are Banach space.

Proof. We give the proof only for $\tilde{W}^1(G \times S \times I)$, as the spaces $\tilde{W}_{\pm}^1(G \times S \times I)$ are handled similarly. If $\{\psi_n\}$ is a Cauchy sequence in $\tilde{W}^1(G \times S \times I)$, then $\psi_n \rightarrow \psi$ in $W^1(G \times S \times I)$, $\gamma(\psi_n) \rightarrow g$ in $T^1(\Gamma)$, thus $\gamma_{\pm}(\psi_n) \rightarrow \gamma_{\pm}(\psi)$ and $\gamma(\psi_n)|_{\Gamma_{\pm}} \rightarrow g|_{\Gamma_{\pm}}$ in $L_{\text{loc}}^1(\Gamma_{\pm}, |\omega \cdot \nu| d\sigma d\omega dE)$, and so $g = \gamma(\psi)$, which implies that $\psi \in \tilde{W}^1(G \times S \times I)$. \square

For $v \in \mathcal{D}(\overline{G} \times S \times I)$ and $u \in \tilde{W}^1(G \times S \times I)$ one has the following Green's formula

$$(8) \quad \int_{G \times S \times I} (\omega \cdot \nabla u) v dx d\omega dE + \int_{G \times S \times I} (\omega \cdot \nabla v) u dx d\omega dE = \int_{\partial G \times S \times I} (\omega \cdot \nu) u v d\sigma d\omega dE$$

which is obtained from the Stokes' Theorem for $u, v \in \mathcal{D}(\overline{G} \times S \times I)$, and then by the limiting process for general $v \in \mathcal{D}(\overline{G} \times S \times I)$ and $u \in \tilde{W}^1(G \times S \times I)$. Similarly, one deduces from Stokes' theorem the following special case of it that holds for $u \in \tilde{W}^1(G \times S \times I)$,

$$(9) \quad \int_{G \times S \times I} (\omega \cdot \nabla u) dx d\omega dE = \int_{\partial G \times S \times I} u (\omega \cdot \nu) d\sigma d\omega dE.$$

As a straightforward application of this formula, we have another trace theorem which we shall need later on (cf. [13] Théorème de trace 2, [16] Lemma 2.1, or [19] Theorem 1, p. 252).

Theorem 2.6 For $\psi \in \tilde{W}_\pm^1(G \times S \times I)$, we have

$$\|\gamma_\mp(\psi)\|_{T^1(\Gamma_\mp)} \leq \|\psi\|_{\tilde{W}_\pm^1(G \times S \times I)}.$$

Proof. We consider here the case $\psi \in \tilde{W}_+(G \times S \times I)$, as the other case is handled analogously. From (9) and the fact that Γ_0 is zero-measurable, we have

$$\begin{aligned} \|\gamma_+(\psi)\|_{T^1(\Gamma_+)} - \|\gamma_-(\psi)\|_{T^1(\Gamma_-)} &= \int_{\Gamma_+} |\psi| |\omega \cdot \nu| d\sigma d\omega dE - \int_{\Gamma_-} |\psi| |\omega \cdot \nu| d\sigma d\omega dE \\ &= \int_{\Gamma_+} |\psi| (\omega \cdot \nu) d\sigma d\omega dE + \int_{\Gamma_-} |\psi| (\omega \cdot \nu) d\sigma d\omega dE = \int_{\partial G \times S \times I} |\psi| (\omega \cdot \nu) d\sigma d\omega dE \\ &= \int_{G \times S \times I} \omega \cdot \nabla |\psi| d\sigma d\omega dE, \end{aligned}$$

from which, by taking into account that $\omega \cdot \nabla |\psi| = \text{sgn}(\psi)(\omega \cdot \nabla \psi)$ a.e. on $G \times S \times I$ (cf. the proof of Theorem 2.3), we have

$$\begin{aligned} \|\gamma_-(\psi)\|_{T^1(\Gamma_-)} &\leq \|\gamma_+(\psi)\|_{T^1(\Gamma_+)} + \int_{G \times S \times I} |\omega \cdot \nabla |\psi|| d\sigma d\omega dE \\ &\leq \|\gamma_+(\psi)\|_{T^1(\Gamma_+)} + \|\omega \cdot \nabla \psi\|_{L^1(G \times S \times I)}. \end{aligned}$$

This completes the proof since the right hand side is clearly less than $\|\psi\|_{\tilde{W}_+^1(G \times S \times I)}$. \square

In particular, we have as sets the equalities

$$\tilde{W}^1(G \times S \times I) = \tilde{W}_+^1(G \times S \times I) = \tilde{W}_-^1(G \times S \times I).$$

Moreover, these spaces are equivalent as normed spaces, with their respective norms introduced above, since for all $\psi \in \tilde{W}^1(G \times S \times I)$,

$$\frac{1}{2} \|\psi\|_{\tilde{W}_\mp^1(G \times S \times I)} \leq \|\psi\|_{\tilde{W}_\pm^1(G \times S \times I)} \leq \|\psi\|_{\tilde{W}^1(G \times S \times I)} \leq 2 \|\psi\|_{\tilde{W}_\mp^1(G \times S \times I)}.$$

Remark 2.7 A. Similarly one can define the spaces $W^p(G \times S \times I)$, $T^p(\Gamma_-)$ and so on for any $1 \leq p < \infty$.

B. In the above we could replace the space $W^1(G \times S \times I)$ with a more general (weighted) space

$$W_\rho^1(G \times S \times I) = \{\psi \in L^1(G \times S \times I) \mid \rho(\omega, E) \omega \cdot \nabla \psi \in L^1(G \times S \times I)\}$$

where ρ is a positive measurable function (cf. Section 6 where $\rho = \sqrt{E}$). Similar note is valid for any $1 \leq p < \infty$. We omit these generalizations here.

3. SOLVING THE CONVECTION EQUATION BY THE METHOD OF CHARACTERISTICS

3.1. On the Escape Time Map. In the following we need the concept of "escape time" $t(x, \omega)$ where $x \in G$ and $\omega \in S$. We define for $(x, \omega) \in G \times S$,

$$\begin{aligned} (10) \quad t(x, \omega) &= t_-(x, \omega) := \inf\{s > 0 \mid x - s\omega \notin G\} \\ &= \sup\{t > 0 \mid x - s\omega \in G \text{ for all } 0 < s < t\}. \end{aligned}$$

For some simple cases this mapping t can be given explicitly.

We give a simple example in which t can be computed explicitly.

Example 3.1 Let G be the ball $B(0, r) \subset \mathbb{R}^3$. Suppose that $x \in G$. We find that the point $y = x - s\omega$ belongs to ∂G exactly when $\|x - s\omega\| = r$. This means that

$$(11) \quad \|x\|^2 - 2s \langle x, \omega \rangle + s^2 = r^2.$$

The solution of (11) is

$$s = \langle x, \omega \rangle \pm \sqrt{\langle x, \omega \rangle^2 + r^2 - \|x\|^2}.$$

Since $t(x, \omega)$ is positive we have

$$t(x, \omega) = \langle x, \omega \rangle + \sqrt{\langle x, \omega \rangle^2 + r^2 - \|x\|^2}.$$

Note that the discriminant appearing in the expression of $t(x, \omega)$ is always positive for $x \in G$. Hence $t \in C^\infty(G \times S)$. We also remark that for $t(x, \omega)$ is defined for $y \in \partial G$ and $t(y, \omega) = 0$, $y \in \partial G$. Hence we see that $t \in C(\overline{G} \times S)$.

As in Example 3.1 one sees generally that

$$(12) \quad t(x, \omega) = \langle x, \omega \rangle \pm \sqrt{\langle x, \omega \rangle^2 + \|y\|^2 - \|x\|^2}$$

where $y = x - t(x, \omega)\omega \in \partial G$. By elementary geometric considerations one finds that the discriminant in the expression (12) is nonnegative for $x \in G$. In the case when G is convex (and bounded) and when it has C^1 -boundary the mapping $t : \overline{G} \times S \rightarrow [0, \infty[$ is continuous and it has continuous partial derivatives $\frac{\partial t}{\partial x_j}$ in $G \times S$ (see Prop. 3.7 below). In the case where G is convex $t(x, \omega)$ is the unique number s such that $y = x - t(x, \omega)\omega \in \partial G$.

We record here a simple general lemma.

Lemma 3.2 (i) For all $(x, \omega) \in G \times S$, one has $x - t(x, \omega)\omega \in \partial G$.
(ii) For every $(x, \omega) \in G \times S$ for which $y := x - t(x, \omega)\omega$ is a regular point of ∂G , it holds $\omega \cdot \nu(y) \leq 0$.

Proof. (i) By the first line (10), one can choose a decreasing sequence of positive numbers (s_n) such that $s_n \rightarrow t(x, \omega)$ and $x - s_n\omega \notin G$. As G is open, one has in the limit that $x - t(x, \omega)\omega \notin G$. Similarly, choosing an increasing sequence (t_n) of strictly positive numbers such that $t_n \rightarrow t(x, \omega)$, by the second line in (10) we have $x - t_n\omega \in G$, and therefore $x - t(x, \omega)\omega \in \overline{G}$.

(ii) We argue by contradiction. Suppose that $y = x - t(x, \omega)\omega$ is a regular point of ∂G but $\omega \cdot \nu(y) > 0$. Then as $\nu(y)$ points outward from G , we necessarily have $y + \tau\omega \notin G$ for all small enough $\tau > 0$, i.e. $x - (t(x, \omega) - \tau)\omega \notin G$, which contradicts the above (inf-)definition of $t(x, \omega) = t_-(x, \omega)$. \square

For the needs of the next proposition, we recall the concept of lower and upper semi-continuity of a mapping, as well as a standard result regarding the existence of supports for a convex (open) subset C of \mathbb{R}^n .

Let X be a metric space and let $f : A \rightarrow \mathbb{R}$, $A \subset X$ be a mapping. Recall that f is lower semi-continuous at $x_0 \in A$ if

$$\liminf_{x \rightarrow x_0} f(x) \geq f(x_0).$$

Similarly f is upper semi-continuous at $x_0 \in A$ if

$$\limsup_{x \rightarrow x_0} f(x) \leq f(x_0).$$

Proposition 3.3 Let $C \subset \mathbb{R}^n$ be an open convex set and let $y \in \partial C$. Then there exists a $\lambda = \lambda_y \in \mathbb{R}^n$ such that $\lambda \cdot (x - y) < 0$ for all $x \in C$.

We call this $\lambda \in \mathbb{R}^n$ a *support* of C at $y \in \partial C$.

Proof. We will prove here a bit more than stated above, namely that for every $y \notin C$ (which is the case if $y \in \partial C$), there exist λ such that $\lambda \cdot (x - y) < 0$ for all $x \in C$.

Observe first that it is enough to prove this in the case $y = 0$, since otherwise one can simply replace C with $C - y = \{x - y \mid x \in C\}$.

In the first place, we assume that $0 \notin \overline{C}$. As \overline{C} is closed, there exists $y \in \overline{C}$ such that $\|y\| = \min\{\|x\| \mid x \in \overline{C}\}$. If $x \in C$ we have by convexity $sx + (1 - s)y \in \overline{C}$ for all $s \in [0, 1]$, from which

$$\|y\|^2 \leq \|sx + (1 - s)y\|^2 = s^2\|x\|^2 + (1 - s)^2\|y\|^2 + 2s(1 - s)x \cdot y,$$

i.e.

$$2s(1 - s)x \cdot (-y) \leq s^2(\|x\|^2 + \|y\|^2) - 2s\|y\|^2.$$

Setting $\lambda := -y$ and letting $s > 0$ tend to zero, we get

$$x \cdot \lambda \leq \lim_{s \rightarrow 0^+} \frac{s(\|x\|^2 + \|y\|^2) - 2\|y\|^2}{2(1 - s)} = -\|\lambda\|^2.$$

Because $0 \notin \overline{C}$, we have $\lambda = -y \neq 0$ and thus $x \cdot \lambda < 0$. Since $x \in C$ was arbitrary, this proves the claim in this special case, i.e. when $0 \notin \overline{C}$.

It remains to consider the case where $0 \in \partial C$. Let (x_n) be a sequence in the complement of \overline{C} that converges to 0 when $n \rightarrow \infty$. Choose a sequence (λ_n) in \mathbb{R}^n , corresponding to x_n as above, such that $\lambda_n \cdot x \leq 0$ for all $x \in C$. We may normalize these vectors λ_n by replacing them by $\frac{\lambda_n}{\|\lambda_n\|}$ i.e. assume that $\|\lambda_n\| = 1$. But then they lie on the compact unit sphere S^{n-1} of \mathbb{R}^n , and thus we may extract a subsequence (λ_{n_i}) converging to $\lambda \in S^{n-1}$ as $i \rightarrow \infty$. If $x \in C$, then $\lambda_{n_i} \cdot x \leq 0$ for all i implies that $\lambda \cdot x \leq 0$ for all $x \in C$ as well.

It remains to show that the above inequality is actually a strict inequality. Indeed, given $x \in C$, the assumption that C is open, implies that $x + \epsilon\lambda \in C$ for a small enough $\epsilon > 0$. But then by what we just proved, $\lambda \cdot (x + \epsilon\lambda) \leq 0$, i.e.

$$\lambda \cdot x \leq -\epsilon\|\lambda\|^2, \quad \forall x \in C,$$

which, since $\epsilon > 0$ and $\|\lambda\|^2 > 0$ implies that $\lambda \cdot x < 0$ as claimed. This completes the proof. \square

Remark 3.4 As is well known, above proposition is actually true in any (possibly infinite dimensional) Hilbert space. Moreover, it can be verified using the above proof with the exception that one must recall that (a) the existence of (a unique) y such that $\overline{y} = \{\|x\| \mid x \in \overline{C}\}$ remains true in this more general setting, because \overline{C} is convex and closed, and (b) that $\|\lambda_n\| = 1$ for all n implies that a subsequence λ_{n_i} converges *weakly* to some λ . Alternatively, it can be seen as a simple corollary of the Hahn-Banach theorem and Riesz representation theorems. However, here we do not need this result in such a generality.

In the next two propositions we formulate the basic continuity and differentiability properties of the escape time t , respectively.

Proposition 3.5 The escape time $t(x, \omega)$ has the following properties:

- (i) Function $t(x, \omega)$ is lower semi-continuous on $G \times S$.
- (ii) Function $t(x, \omega)$ is continuous on $G \times S$ if and only if G is convex. In addition, in this case, for all $(x_0, \omega_0) \in G \times S$ if $y_0 = x_0 - t(x_0, \omega_0)\omega_0$, we have

$$(13) \quad \lim_{(x, \omega) \rightarrow (y_0, \omega_0)} t(x, \omega) = 0.$$

Proof. (i) We assume that $t(x, \omega)$ is not lower semi-continuous, and show that this leads to a contradiction, thus proving the claim. Indeed, if this is the case, there is a sequence (x_n, ω_n) in $G \times S$ converging to $(x, \omega) \in G \times S$ and $\bar{t} > 0$ such that $t(x, \omega) > \bar{t} \geq \liminf_{n \rightarrow \infty} t(x_n, \omega_n)$. Since $t(x_n, \omega_n)$ belongs to a bounded set $[0, \bar{t}]$, there is a subsequence of (x_n, ω_n) , which we still denote by (x_n, ω_n) , such that $t(x_n, \omega_n)$ converges to a number $t_0 \in [0, \bar{t}]$.

But then the limit $\lim_{n \rightarrow \infty} (x_n - t(x_n, \omega_n)\omega_n)$ exists and equals $x - t_0\omega \in \partial G$, which by the definition of $t(x, \omega)$ implies that $t(x, \omega) \leq t_0$. This gives us a contradiction since

$$t(x, \omega) \leq t_0 = \lim_{n \rightarrow \infty} t(x_n, \omega_n) \leq \bar{t} < t(x, \omega).$$

(ii) Assume first that G is convex. Let $(x, \omega) \in G \times S$ and choose any $\alpha \in \mathbb{R}$ and $\lambda \in \mathbb{R}^3$ such that $\lambda \cdot z < \alpha$ for all $z \in G$ and $\lambda \cdot (x - t(x, \omega)\omega) = \alpha$, i.e. $\lambda \cdot x - \alpha = t(x, \omega)\lambda \cdot \omega$. This is possible by Proposition 3.3, choosing $y := x - t(x, \omega)\omega \in \partial G$ there, and writing $\alpha := \lambda \cdot y$.

Notice that because $t(x, \omega) > 0$ and $t(x, \omega)\lambda \cdot \omega = \lambda \cdot x - \alpha < 0$, we must have $\lambda \cdot \omega < 0$. Then if (x_n, ω_n) is any sequence in $G \times S$ converging to (x, ω) , one has

$$\alpha \geq \lambda \cdot (x_n - t(x_n, \omega_n)\omega_n) = \lambda \cdot x_n - t(x_n, \omega_n)\lambda \cdot \omega_n$$

i.e.

$$t(x_n, \omega_n)\lambda \cdot \omega_n \geq \lambda \cdot x_n - \alpha,$$

and therefore

$$\limsup_{n \rightarrow \infty} t(x_n, \omega_n) \leq \frac{\lambda \cdot x - \alpha}{\lambda \cdot \omega} = t(x, \omega).$$

This proves the upper semi-continuity of t , which combined with the result of the case (i) shows the continuity of t on G .

In the opposite direction, let us then demonstrate that the convexity of G follows from the continuity of t on $G \times S$. Indeed, if G is not convex, there are $x, y \in G$ such that the line $\ell_{x,y} := \{x + t(y - x) \mid x \in [0, 1]\}$ between them is not completely contained in G . Since G is open and connected, there is a path $\gamma : [0, 1] \rightarrow G$ such that $\gamma(0) = x$, $\gamma(1) = y$ and $\gamma(s) \neq x$ for all $s \in]0, 1]$. Define $s_0 \in \mathbb{R}$ to be the infimum of $s \in [0, 1]$ such that $\ell_{x, \gamma(s)} \not\subset G$. Clearly, $s_0 > 0$ and $\ell_{x, \gamma(s_0)} \not\subset G$. We let $s_n \in]0, 1]$ be an increasing sequence whose limit is s_0 , and define $\omega_n := \frac{x - \gamma(s_n)}{\|\gamma(s_n) - x\|}$, $\omega_0 := \frac{x - \gamma(s_0)}{\|\gamma(s_0) - x\|}$. But then for all n and $s \in [0, \|\gamma(s_n) - x\|]$ we have $x - s\omega_n \in G$, and therefore $t(x, \omega_n) \geq \|\gamma(s_n) - x\|$. On the other hand, since $\ell_{x, \gamma(s_0)} \not\subset G$ and $\gamma(s_0) \in G$, one has $t(x, \omega_0) < \|\gamma(s_0) - x\|$. Finally, because $(x, \omega_n) \rightarrow (x, \omega_0)$, we have

$$\limsup_{n \rightarrow \infty} t(x, \omega_n) \geq \limsup_{n \rightarrow \infty} \|\gamma(s_n) - x\| = \|\gamma(s_0) - x\| > t(x, \omega_0),$$

and thus, we conclude that t is not upper semi-continuous on $G \times S$. This completes the proof of the first part of (ii).

For the second part, let $(x_0, \omega_0) \in G \times S$ and $y_0 = x_0 - t(x_0, \omega_0)\omega_0$. As $y_0 \in \partial G$ by Lemma 3.2, there exists by Proposition 3.3 a number $\alpha \in \mathbb{R}$ and a vector $\lambda \in \mathbb{R}^3$ such that $\lambda \cdot y < \alpha$ for all $y \in G$ and $\lambda \cdot y_0 = \alpha$.

Therefore, as $x_0 \in G$, we have $\lambda \cdot x_0 < \alpha$ and since $t_0 := t(x_0, \omega_0) > 0$, we deduce that $\lambda \cdot \omega_0 = t_0^{-1}(\lambda \cdot x_0 - \alpha) < 0$. Then if (x_n, ω_n) is a sequence in $G \times S$ that converges to (y_0, ω_0) in $\mathbb{R}^3 \times S$, we have like earlier, $t(x_n, \omega_n)\lambda \cdot \omega_n \geq \lambda \cdot x_n - \alpha$. Combining this with the inequality $\lambda \cdot \omega_0 < 0$ allows us to conclude

$$\limsup_{n \rightarrow \infty} t(x_n, \omega_n) \leq \frac{\lambda \cdot y_0 - \alpha}{\lambda \cdot \omega_0} = 0,$$

where in the last step we used again the equality $\lambda \cdot y_0 = \alpha$. The proof of case (ii) is finished. \square

Remark 3.6 The results of Proposition 3.5 remain true with the given proof if G is an arbitrary open bounded convex subset of \mathbb{R}^3 , i.e. it does not necessarily have to have piecewise C^1 -boundary.

In particular, due to lower semicontinuity (case (i) of the above proposition) the escape time t is a Lebesgue-measurable map on $G \times S$.

Proposition 3.7 The mapping $t : G \times S \rightarrow \mathbb{R}$ is continuously differentiable on a neighbourhood of every point $(x_0, \omega_0) \in G \times S$ for which $\omega \cdot \nu(y_0) < 0$, where $y_0 = x_0 - t(x_0, \omega_0)\omega_0 \in \partial G$ and where y_0 is a regular point of ∂G . Moreover, in this case (13) holds at the point $(y_0, \omega_0) \in \Gamma_-$ and

$$(14) \quad \omega_0 \cdot (\nabla t)(x_0, \omega_0) = 1.$$

Proof. Let $(x_0, \omega_0) \in G \times S$ be such that $y_0 = x_0 - t(x_0, \omega_0)\omega_0$ is a regular point of ∂G and that $\omega_0 \cdot \nu(y_0) < 0$. Choose C^1 -diffeomorphism $H : D \rightarrow V$ from an open subset $D \subset \mathbb{R}^3$ onto an open subset $V \subset \mathbb{R}^3$ containing y_0 such that $V \cap \overline{G} = H(D_+)$, with $D_+ = \{(x_1, x_2, x_3) \in D \mid x_3 \geq 0\}$ and $V \cap \partial G = H(D_0)$ where $D_0 = \{(x_1, x_2, 0) \in D\}$, which we implicitly identify with the obvious subset of \mathbb{R}^2 . Such a H exists since y_0 was assumed to be a regular point of ∂G . Define

$$F : D_0 \times \mathbb{R} \times S \rightarrow \mathbb{R}^3 \times S; \quad F(u, s, \omega) = (H(u, 0) + s\omega, \omega),$$

where $u = (u_1, u_2) \in D_0$, $s \in \mathbb{R}$, $\omega \in S$. Clearly F is C^1 , and if $y_0 = H(u_0, 0)$ and $t_0 = t(x_0, \omega_0)$, we have $F(u_0, t_0, \omega_0) = (x_0, \omega_0)$. Moreover, identifying $T_{u_0}D_0$ with \mathbb{R}^2 as well,

$$DF(u_0, t_0, \omega_0)(v, r, \theta) = (DH(u_0, 0)v + r\omega_0 + t_0\theta, \theta), \quad (v, r, \theta) \in \mathbb{R}^2 \times \mathbb{R} \times T_{\omega_0}S,$$

and therefore $DF(u_0, t_0, \omega_0)(v, r, \theta) = 0$ implies

$$\theta = 0 \quad \text{and} \quad DH(u_0, 0)v + r\omega_0 = 0.$$

Using that $DH(u_0, 0)v \in T_{y_0}(\partial G)$, we have furthermore

$$0 = \nu(y_0) \cdot (DH(u_0, 0)v + r\omega_0) = r\nu(y_0) \cdot \omega_0$$

and since $\omega_0 \cdot \nu(y_0) < 0$, that $r = 0$ and finally $v = 0$.

It has thus been shown (by the Inverse Mapping Theorem) that F is a diffeomorphism from a small neighbourhood W of (u_0, t_0, ω_0) onto a neighbourhood U of (x_0, ω_0) . We claim that

$$(15) \quad t(F(u, s, \omega)) = s, \quad \forall (u, s, \omega) \in W.$$

Once this is established, it is clear that t is a C^1 -mapping on U because then

$$t(x, \omega) = \text{pr}_2(F^{-1}(x, \omega)), \quad \forall (x, \omega) \in U,$$

where pr_2 is the projection onto the second factor $D_0 \times \mathbb{R} \times S \rightarrow D_0$.

It suffices to show that we can shrink W around (u_0, t_0, ω_0) such that the (half open) segment $\{H(u, 0) + s\omega \mid 0 < s \leq \tau\}$ lies completely in G for all $(u, \tau, \omega) \in W$. Indeed, once this has been established, (15) follows directly from the definition of t .

To show that such a modification of W is possible, we argue by contradiction. Thus, suppose that there was a sequence (u_n, τ_n, ω_n) in W converging to (u_0, t_0, ω_0) and a sequence of numbers s_n , $0 < s_n \leq \tau_n$, such that $v_n := H(u_n, 0) + s_n\omega_n \notin G$. Taking the numbers s_n to be smaller if necessary, we may assume that $v_n \in \partial G$ for every n . As the sequence (s_n) is bounded, we may pass to a subsequence (s_{n_i}) that converges to some $s' \in [0, t_0]$ (as $\tau_{n_i} \rightarrow t_0$), and because ∂G is closed, we have $\lim_{i \rightarrow \infty} v_{n_i} = H(u_0, 0) + s'\omega_0 \in \partial G$. On the other hand, $H(u_0, 0) = y_0 = x_0 - t_0\omega_0$ and hence the definition of $t_0 = t(x_0, \omega_0)$ implies that $t_0 \leq t_0 - s'$ i.e. $s' = 0$. Thus $v_{n_i} \rightarrow y_0 = H(u_0, 0)$ in \mathbb{R}^3 when $i \rightarrow \infty$.

The boundary ∂G being an embedded submanifold of \mathbb{R}^3 , we have $v_{n_i} \rightarrow y_0$ also in ∂G , and hence for all i big enough, one has $v_{n_i} = H(\tilde{u}_{n_i}, 0)$ for some $\tilde{u}_{n_i} \in D_0$ such that $\tilde{u}_{n_i} \rightarrow u_0$ when $i \rightarrow \infty$.

Computing the differential of F at $(u_0, 0, \omega_0)$ as above, we see that $DF(u_0, 0, \omega_0)(v, r, \theta) = (DH(u_0, 0)v + r\omega_0, \theta)$, from which it is seen that $DF(u_0, 0, \omega_0)$ is invertible, and hence that F is a C^1 -diffeomorphism from an open neighbourhood \tilde{W} of $(u_0, 0, \omega_0)$ onto an open neighbourhood \tilde{U} of $F(u_0, 0, \omega_0) = (y_0, \omega_0)$ in $\mathbb{R}^3 \times S$. But $(\tilde{u}_{n_i}, 0, \omega_{n_i}) \rightarrow (u_0, 0, \omega_0)$, hence for i large enough, points $(\tilde{u}_{n_i}, 0, \omega_{n_i})$ and $(u_{n_i}, s_{n_i}, \omega_{n_i})$ all belong to \tilde{W} . On the other hand,

$$F(u_{n_i}, s_{n_i}, \omega_{n_i}) = (v_{n_i}, \omega_{n_i}) = (H(\tilde{u}_{n_i}, 0), \omega_{n_i}) = F(\tilde{u}_{n_i}, 0, \omega_{n_i}),$$

and thus the injectivity of F on \tilde{W} implies that $(u_{n_i}, s_{n_i}, \omega_{n_i}) = (\tilde{u}_{n_i}, 0, \omega_{n_i})$ for large enough i . In particular $s_{n_i} = 0$ for large i , which contradicts the fact that $s_n > 0$ for all n .

As explained before, this contradiction establishes 15 and concludes our proof of C^1 -differentiability property t as announced in the statement of this proposition.

We shall next demonstrate the limiting property (13). Let (x_n, ω_n) be a sequence in $G \times S$ converging to (y_0, ω_0) , where as before $y_0 = x_0 - t_0(x_0, \omega_0)\omega_0 \in \partial G$. Using the F as defined previously, and setting $y_0 = H(u_0, 0)$, we have as above that $DF(u_0, 0, \omega_0)(v, r, \theta) = (DH(u_0, 0)v + r\omega_0, \theta)$, from which we again deduce that $DF(u_0, 0, \omega_0)$ is invertible, and therefore there exist an open subset $\tilde{W} \subset D_0 \times \mathbb{R} \times S$ containing $(u_0, 0, \omega_0)$ which is mapped diffeomorphically onto an open neighbourhood $\tilde{U} \subset \mathbb{R}^3 \times S$ of (y_0, ω_0) .

Defining u_n, s_n by requiring that $F(u_n, s_n, \omega_n) = (x_n, \omega_n)$, we have $(u_n, s_n, \omega_n) \rightarrow F^{-1}(y_0, \omega_0) = (u_0, 0, \omega_0)$. On the other hand, as $x_n - s_n\omega_n = H(u_n, 0) \in \partial G$, it follows that $t(x_n, \omega_n) \leq s_n$ for all n and therefore

$$\limsup_{n \rightarrow \infty} t(x_n, \omega_n) \leq \lim_{n \rightarrow \infty} s_n = 0.$$

Hence the validity of the limit (13) is demonstrated (since $\liminf_{n \rightarrow \infty} t(x_n, \omega_n) \geq 0$).

Finally, to prove (14), we observe that whenever $|s|$ is small enough, $s \in \mathbb{R}$, it holds that $t(x_0 + s\omega_0, \omega_0) = s + t(x_0, \omega_0)$ and hence

$$\omega_0 \cdot (\nabla t)(x_0, \omega_0) = \frac{d}{ds} \Big|_{s=0} t(x_0 + s\omega_0, \omega_0) = \frac{d}{ds} \Big|_{s=0} (s + t(x_0, \omega_0)) = 1.$$

□

Since Γ_0 has measure zero on $\partial G \times S \times I$, we have the following result (cf. Lemme 2.3.3 in [4]):

Theorem 3.8 The set

$$N_0 := \{(x, \omega, E) \in G \times S \times I \mid \text{either } y \in \partial G \setminus (\partial G)_r, \text{ or } y \in (\partial G)_r \text{ and } \omega \cdot \nu(y) = 0, \\ \text{where } y = x - t(x, \omega)\omega \in \partial G\}$$

has a measure zero in $G \times S \times I$.

Proof. First observe that

$$N_0 \subset P((\tilde{\Gamma}_0 \times \mathbb{R}) \cup ((\partial G \setminus (\partial G)_r) \times S \times I \times \mathbb{R})),$$

where

$$P : \partial G \times S \times I \times \mathbb{R} \rightarrow \mathbb{R}^3 \times S \times I; \quad P(y, \omega, E, t) = (y + t\omega, \omega, E).$$

Since $(\tilde{\Gamma}_0 \times \mathbb{R}) \cup ((\partial G \setminus (\partial G)_r) \times S \times I \times \mathbb{R})$ has measure zero in $\partial G \times S \times I \times \mathbb{R}$ and $\dim(\partial G \times S \times I \times \mathbb{R}) = \dim(\mathbb{R}^3 \times S \times I)$, to prove the theorem, it suffices to show that P is locally Lipschitz-continuous, since then it maps sets of Lebesgue measure zero to sets of Lebesgue measure zero. Indeed, we have

$$\begin{aligned} & d_{\mathbb{R}^3 \times S \times I}(P(y_1, \omega_1, E_1, t_1), P(y_2, \omega_2, E_2, t_2)) \\ &= \|y_1 - y_2\| + \|t_1\omega_1 - t_2\omega_2\| + d_S(\omega_1, \omega_2) + |E_1 - E_2| \\ &\leq \|y_1 - y_2\| + |t_1 - t_2| + |t_1| \|\omega_1 - \omega_2\| + d_S(\omega_1, \omega_2) + |E_1 - E_2| \\ &\leq C_1 d_{\partial G}(y_1, y_2) + |t_1 - t_2| + (1 + |t_1|)C_2 d_S(\omega_1, \omega_2) + |E_1 - E_2|, \end{aligned}$$

where $d_{\partial G}$ and d_S are the (intrinsic) geodesic metrics on ∂G and S , respectively, and $C_1, C_2 > 0$ are some constants coming from the fact that these geodesic metrics are equivalent with the restrictions of metrics of the ambient space \mathbb{R}^3 (recall that ∂G is compact). Finally, for any bounded interval $J \subset \mathbb{R}$ there is a constant $C_3 > 0$ such that the last line in the above inequality is dominated by $C_3 d_{\partial G \times S \times I \times \mathbb{R}}((y_1, \omega_1, E_1, t_1), (y_2, \omega_2, E_2, t_2))$, whenever $t_1, t_2 \in J$. This established the claim. □

3.2. Local Solution Obtained by Lagrange's Method. We consider only the convection of one particle that is, the solution ψ is scalar valued. The vector valued case ($\psi = (\psi_1, \psi_2, \psi_3)$) is then obtained (when required) easily and it is considered in section 3.3.

At first we apply the classical Lagrange's method (the method of characteristics) for the convection equation

$$(16) \quad \omega \cdot \nabla \psi + \lambda \psi = f(x, \omega, E)$$

where $\lambda \in \mathbb{R}$ and $f \in C(\overline{G} \times S \times I)$. We demand that the solution $\psi = \psi(x, \omega, E)$ satisfy the inflow boundary condition

$$(17) \quad \psi(y, \omega, E) = 0, \quad \text{when } (y, \omega, E) \in \partial G_r \times S \times I; \quad \omega \cdot \nu(y) < 0.$$

First, we seek a general solution for the equation (16), which we write as

$$\sum_{j=1}^3 \omega_j \frac{\partial \psi}{\partial x_j} + \lambda \psi = f(x, \omega, E).$$

Denote $(x, \omega, E) = (x_1, x_2, x_3, \omega_1, \omega_2, \omega_3, E)$. Then the augmented system of ordinary differential equations (the system of characteristics) is

$$\begin{aligned} X_1'(s) &= \Omega_1, & \Omega_1'(s) &= 0 \\ X_2'(s) &= \Omega_2, & \Omega_2'(s) &= 0 \\ X_3'(s) &= \Omega_3, & \Omega_3'(s) &= 0 \\ \mathcal{E}'(s) &= 0 \\ \Psi'(s) &= f(X, \Omega, \mathcal{E}) - \lambda \Psi \end{aligned}$$

where we denoted $X = (X_1, X_2, X_3)$, $\Omega = (\Omega_1, \Omega_2, \Omega_3)$.

We have $\Omega_j'(s) = 0$, $\mathcal{E}'(s) = 0$ which implies $\Omega_j(s) = C_j$ (a constant) and $\mathcal{E} = C''$ (a constant). Hence we further get $X_j'(s) = C_j$ and so $X_j(s) = C_j s + C_j'$ where C_j' are constants. Denote $C = (C_1, C_2, C_3)$, $C' = (C_1', C_2', C_3')$. Then

$$\Psi'(s) = f(sC + C', C, C'') - \lambda \Psi$$

whose solutions is

$$(18) \quad \Psi(s) = e^{-\lambda s} \left(C_0 + \int_0^s f(\tau C + C', C, C'') e^{\lambda \tau} d\tau \right),$$

where C_0 is again a constant.

Next we consider (locally) the initial value for the augmented system. It must be of the form $(X(0), \Omega(0), \mathcal{E}(0), \Psi(0)) = \Theta(w)$ where $w \in W \subset \mathbb{R}^6$ and $\Theta : W \rightarrow \mathbb{R}^8$ is the (local) parametrization of the 6-dimensional manifold $\zeta := \Theta(W)$ through which the curve $(X, \Omega, \mathcal{E}, \Psi)$ goes at $s = 0$. Let $h = (h_1, h_2, h_3) : \mathcal{V} \rightarrow \partial G$, $\mathcal{V} \subset \mathbb{R}^2$ (open) be a local parametrization of the boundary ∂G_r . Suppose that $y_0 = h(v_0) \in (\partial G)_r$ such that $\omega_0 \cdot \nu(y_0) = \omega_0 \cdot \nu(h(v_0)) < 0$. Then there exist an open neighbourhood $\mathcal{V}' \subset \mathcal{V}$ and an open neighbourhood $\mathcal{U} \subset \mathbb{R}^3$ such that $\omega \cdot \nu(h(v)) < 0$ for all $(v, \omega) \in \mathcal{V}' \times \mathcal{U}$ (here we exceptionally assume ω belongs to an open subset of \mathbb{R}^3). Hence the local parametrization Θ is

$$\Theta : \mathcal{V}' \times \mathcal{U} \times \Delta \rightarrow \mathbb{R}^8; \quad \Theta(w) = (h(v), \omega, E, 0), \quad w = (v, \omega, E)$$

where $\Delta \subset I$.

The initial condition is

$$(X(0), \Omega(0), \mathcal{E}(0), \Psi(0)) = \Theta(w) = (h(v), \omega, E, 0)$$

which is equivalent to

$$(19) \quad X(0) = h(v), \quad \Omega(0) = \omega, \quad \mathcal{E}(0) = E, \quad \Psi(0) = 0.$$

Taking into account the above obtained general solutions, the condition (19) means that $C_0 = 0$, $C' = h(v)$, $C = \omega$, $C'' = E$ and then

$$(20) \quad X(s) := X_{(v, \omega, E)}(s) = s\omega + h(v), \quad \Omega(s) := \Omega_{(v, \omega, E)}(s) = \omega, \quad \mathcal{E}(s) := \mathcal{E}_{(v, \omega, E)}(s) = E$$

and

$$(21) \quad \Psi(s) := \Psi_{(v, \omega, E)}(s) = e^{-\lambda s} \int_0^s f(\tau\omega + h(v), \omega, E) e^{\lambda \tau} d\tau.$$

The Lagrange's method proceeds as follows. We denote

$$(22) \quad X(s) = x, \quad \Omega(s) = \omega, \quad \mathcal{E}(s) = E$$

from which we must eliminate s , v , $(\omega$ and $E)$. We find that the equations (22) mean that

$$(23) \quad h(v) = x - s\omega \in \partial G \text{ or } v = h^{-1}(x - s\omega).$$

Since $x - s\omega = h(v) \in \partial G$ the definition of $t(x, \omega)$ implies that $s = t(x, \omega)$ in (23). Hence the solution ψ

$$(24) \quad \psi(x, \omega, E) = \Psi_{(h^{-1}(x-s\omega), \omega, E)}(t(x, \omega))$$

$$(25) \quad = e^{-\lambda t(x, \omega)} \int_0^{t(x, \omega)} f(\tau\omega + x - t(x, \omega)\omega, \omega, E) e^{\lambda\tau} d\tau$$

$$(26) \quad = \int_0^{t(x, \omega)} f(x - \tau\omega, \omega, E) e^{-\lambda\tau} d\tau.$$

The applied Lagrange's method gives (locally) a unique continuous solution (for which $\frac{\partial\psi}{\partial x_j}$ are continuous) when initial value manifold ζ is not characteristic at $\Theta(w_0)$ for the convection equation. This means that at the given point $(x_0, \omega_0, E_0, 0) = (h(v_0), \omega_0, E_0, 0) = \Theta(w_0) \in \zeta$ one must have

$$(27) \quad \det \begin{pmatrix} \partial_1 \theta(w_0) \\ \vdots \\ \partial_6 \theta(w_0) \\ a(x_0, \omega_0, E_0) \end{pmatrix} \neq 0$$

where $\theta(w) := (h(v), \omega, E)$ and $a(x, \omega, E) := (-\omega_1, -\omega_2, -\omega_3, 0, 0, 0, 0)$. Hence

$$(28) \quad \det \begin{pmatrix} \partial_1 h_1(v_0) & \partial_1 h_2(v_0) & \partial_1 h_3(v_0) & 0 & 0 & 0 & 0 \\ \partial_2 h_1(v_0) & \partial_2 h_2(v_0) & \partial_2 h_3(v_0) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ \omega_{10} & \omega_{20} & \omega_{30} & 0 & 0 & 0 & 0 \end{pmatrix} \neq 0$$

that is

$$\omega_{10} \det \begin{pmatrix} \partial_1 h_2 & \partial_1 h_3 \\ \partial_2 h_2 & \partial_2 h_3 \end{pmatrix} - \omega_{20} \det \begin{pmatrix} \partial_1 h_1 & \partial_1 h_3 \\ \partial_2 h_1 & \partial_2 h_3 \end{pmatrix} + \omega_{30} \det \begin{pmatrix} \partial_1 h_1 & \partial_1 h_2 \\ \partial_2 h_1 & \partial_2 h_2 \end{pmatrix} \neq 0,$$

where partial derivatives $\partial_i h_j$ are evaluated at v_0 . Since the normal $\nu(y_0)$ of the surface ∂G_r at $y_0 := h(v_0)$ is parallel to

$$\begin{pmatrix} \det \begin{pmatrix} \partial_1 h_2(v_0) & \partial_1 h_3(v_0) \\ \partial_2 h_2(v_0) & \partial_2 h_3(v_0) \end{pmatrix}, -\det \begin{pmatrix} \partial_1 h_1(v_0) & \partial_1 h_3(v_0) \\ \partial_2 h_1(v_0) & \partial_2 h_3(v_0) \end{pmatrix}, \det \begin{pmatrix} \partial_1 h_1(v_0) & \partial_1 h_2(v_0) \\ \partial_2 h_1(v_0) & \partial_2 h_2(v_0) \end{pmatrix} \end{pmatrix} \\ = (\partial_1 h \times \partial_2 h)(v_0)$$

the condition (28) is equivalent to $\omega_0 \cdot \nu(y_0) \neq 0$ which is satisfied on the manifold ζ where $\omega \cdot \nu(h(v)) < 0$. Hence the obtained solution ψ exists locally and it is unique.

Remark 3.9 The above expressed method of characteristics needs only the condition $\omega_0 \cdot \nu(y_0) \neq 0$ to guarantee the existence of the unique *local* solution such that $\frac{\partial\psi}{\partial x_j}$ are continuous.

Remark 3.10 Here we give formally a shorter argument for the derivation of the explicit form of the solution to (16):

$$\frac{d}{ds}\psi(x - s\omega, \omega, E) = -\omega \cdot \nabla \psi(x - s\omega, \omega, E) = \lambda\psi(x - s\omega, \omega, E) - f(x - s\omega, \omega, E).$$

Write $\Psi(s) = \psi(x - s\omega, \omega, E)$, $F(s) = f(x - s\omega, \omega, E)$, and we have

$$\Psi'(s) - \lambda\Psi(s) = -F(s),$$

i.e.

$$\frac{d}{ds}(e^{-\lambda s}\Psi(s)) = -e^{-\lambda s}F(s),$$

from which

$$\Psi(s) = e^{\lambda s}\left(\Psi(0) - \int_0^s e^{-\lambda\tau}F(\tau)d\tau\right),$$

or

$$\psi(x - s\omega, \omega, E) = e^{\lambda s}\left(\psi(x, \omega, E) - \int_0^s e^{-\lambda\tau}f(x - \tau\omega, \omega, E)d\tau\right).$$

Letting $s = t(x, \omega)$, we therefore obtain

$$\psi(x, \omega, E) = e^{-\lambda t(x, \omega)}\psi(x - t(x, \omega)\omega, \omega, E) + \int_0^{t(x, \omega)} e^{-\lambda\tau}f(x - \tau\omega, \omega, E)d\tau,$$

where the first term on the right hand side vanishes, because of the assumption that $\psi = 0$ on Γ_- .

3.3. Global Solution Given by the Method of Characteristics. The section 3.1 suggests that the solution for the convection equation (for $\lambda \in \mathbb{R}$)

$$(29) \quad \omega \cdot \nabla \psi + \lambda\psi = f(x, \omega, E)$$

be

$$(30) \quad \psi(x, \omega, E) = \int_0^{t(x, \omega)} f(x - s\omega, \omega, E)e^{-\lambda s} ds.$$

In the following we denote

$$D := (G \times S \times I) \setminus N_0,$$

where N_0 is Lebesgue zero measurable set given in Theorem 3.8.

Theorem 3.11 Suppose that $f \in C(\overline{G} \times S \times I)$ is such that $\frac{\partial f}{\partial x_j} \in C(\overline{G} \times S \times I)$. Then (30) is the unique solution of the equation (29) in D satisfying the inflow boundary condition $\psi(y, \omega, E) = 0$ for $(y, \omega, E) \in \Gamma_-$ where $y := x - t(x, \omega)\omega$, $x \in D$ (that is, ψ is the classical solution in D).

Proof. Since $f \in C(\overline{G} \times S \times I)$ the expression (30) is defined for all $(x, \omega, E) \in \overline{G} \times S \times I$. Define

$$F(x, \omega, E, t) = \int_0^t f(x - s\omega, \omega, E)e^{-\lambda s} ds, \quad (x, \omega, E) \in D, \quad t \in [0, t(x, \omega)].$$

Then for $(x, \omega, E) \in D$,

$$(31) \quad \psi(x, \omega, E) = F(x, \omega, E, t(x, \omega))$$

and so

$$(32) \quad \frac{\partial \psi}{\partial x_j} = \frac{\partial F}{\partial x_j}(x, \omega, E, t(x, \omega)) + \frac{\partial F}{\partial t}(x, \omega, E, t(x, \omega)) \frac{\partial t}{\partial x_j}(x, \omega).$$

Hence (recall that by assumption $\frac{\partial f}{\partial x_j} \in C(\overline{G} \times S \times I)$)

$$(33) \quad \frac{\partial \psi}{\partial x_j} = \int_0^{t(x, \omega)} \frac{\partial f}{\partial x_j}(x - s\omega, \omega, E) e^{-\lambda s} ds + f(x - t(x, \omega)\omega, \omega, E) e^{-\lambda t(x, \omega)} \frac{\partial t}{\partial x_j}(x, \omega).$$

Hence we see that $\frac{\partial \psi}{\partial x_j}(x, \omega, E)$ exists on D and

$$(34) \quad \omega \cdot \nabla \psi = \int_0^{t(x, \omega)} \omega \cdot \nabla_x f(x - t\omega, \omega, E) e^{-\lambda t} dt$$

$$(35) \quad + f(x - t(x, \omega)\omega, \omega, E) e^{-\lambda t(x, \omega)} \omega \cdot (\nabla_x t)(x, \omega).$$

Using Eq. (14) i.e. $\omega \cdot (\nabla_x t)(x, \omega) = 1$ and the basic fact that

$$\frac{d}{ds} f(x - s\omega, \omega, E) = -\omega \cdot \nabla_x f(x - s\omega, \omega, E),$$

we can simplify the above formula as follows:

$$\begin{aligned} \omega \cdot \nabla \psi &= \int_0^{t(x, \omega)} -\left(\frac{d}{ds} f(x - s\omega, \omega, E)\right) e^{-\lambda s} ds + f(x - t(x, \omega)\omega, \omega, E) e^{-\lambda t(x, \omega)} \\ &= -f(x - t(x, \omega)\omega, \omega, E) e^{-\lambda t(x, \omega)} + f(x, \omega, E) \\ &\quad - \lambda \int_0^{t(x, \omega)} f(x - s\omega, \omega, E) e^{-\lambda s} ds + f(x - t(x, \omega)\omega, \omega, E) e^{-\lambda t(x, \omega)} \\ &= f(x, \omega, E) - \lambda F(x, \omega, E, t(x, \omega)) \\ &= f(x, \omega, E) - \lambda \psi. \end{aligned}$$

We thus see that the convection equation holds.

For $y \in \Gamma_-$ given in the assertion we have by Proposition 3.7 $t(y, \omega) = 0$ and then $\psi(y, \omega, E) = 0$ for the inflow boundary points given in the theorem. This finishes the proof. \square

By applying the similar methods as above we get the following theorems (cf. [19], p. 244-246).

Theorem 3.12 Suppose that $f \in C(\overline{G} \times S \times I)$ such that $\frac{\partial f}{\partial x_j} \in C(\overline{G} \times S \times I)$, and let $\Sigma \in C(\overline{G} \times S \times I)$ such that $\frac{\partial \Sigma}{\partial x_j} \in C(\overline{G} \times S \times I)$, $j = 1, 2, 3$. Then the unique (classical) solution of the equation

$$(36) \quad \omega \cdot \nabla \psi + \Sigma(x, \omega, E) \psi = f(x, \omega, E) \quad \text{in } D$$

satisfying the homogeneous inflow boundary condition

$$(37) \quad \psi(y, \omega, E) = 0 \quad \text{for } (y, \omega, E) \in \Gamma_-$$

is given by

$$(38) \quad \psi(x, \omega, E) = \int_0^{t(x, \omega)} e^{-\int_0^t \Sigma(x - s\omega, \omega, E) ds} f(x - t\omega, \omega, E) dt.$$

Theorem 3.13 Suppose that $g \in C(\Gamma_-)$ such that $\frac{\partial g}{\partial \bar{y}_i} \in C(\Gamma_-)$, $i = 1, 2$, where $\frac{\partial}{\partial \bar{y}_i}$ denotes any local basis of the tangent space of $(\partial G)_r$ (and $\frac{\partial g}{\partial \bar{y}_i} \in C(\Gamma_-)$ is to be understood in a local sense), and $\Sigma \in C(\bar{G} \times S \times I)$ such that $\frac{\partial \Sigma}{\partial x_j} \in C(\bar{G} \times S \times I)$, $j = 1, 2, 3$. Then the unique (classical) solution of the equation

$$(39) \quad \omega \cdot \nabla \psi + \Sigma(x, \omega, E) \psi = 0 \text{ in } D$$

satisfying the inhomogeneous inflow boundary condition

$$(40) \quad \psi(y, \omega, E) = g(y, \omega, E) \text{ for } (y, \omega, E) \in \Gamma_-$$

is given by

$$(41) \quad \psi(x, \omega, E) = e^{-\int_0^{t(x, \omega)} \Sigma(x - s\omega, \omega, E) ds} g(x - t(x, \omega)\omega, \omega, E).$$

Proof. We denote $B : G \times S \times I \rightarrow \partial G$; $B(x, \omega, E) = x - t(x, \omega)\omega$, which by Proposition 3.7 is C^1 -smooth on D . It then follows from the considerations in section 3.1, that $(x, \omega, E) \mapsto (B(x, \omega, E), \omega, E)$ is C^1 -map with respect to x from D into Γ_- , and hence, by the regularity assumptions imposed on g , that the partial derivatives $\frac{\partial}{\partial x_i} g(B(x, \omega, E), \omega, E)$ exist and are continuous on D .

Taking ψ to be defined by Eq. (41), which can be written as

$$(42) \quad \psi(x, \omega, E) = e^{-\int_0^{t(x, \omega)} \Sigma(x - s\omega, \omega, E) ds} g(B(x, \omega, E), \omega, E),$$

we have on D ,

$$\begin{aligned} & \nabla_x \psi(x, \omega, E) \\ &= \psi(x, \omega, E) \left(-\Sigma(x - t(x, \omega)\omega, \omega, E) (\nabla_x t)(x, \omega) - \int_0^{t(x, \omega)} (\nabla_x \Sigma)(x - s\omega, \omega, E) ds \right) \\ & \quad + e^{-\int_0^{t(x, \omega)} \Sigma(x - s\omega, \omega, E) ds} \nabla_x (g(B(x, \omega, E), \omega, E)). \end{aligned}$$

We shall take an inner product of this formula with ω . To this end, recall that $\omega \cdot (\nabla_x t)(x, \omega) = 1$ by (14), and notice that $\omega \cdot (\nabla_x \Sigma)(x - s\omega, \omega, E) = -\frac{d}{ds} \Sigma(x - s\omega, \omega, E)$. Moreover, for all s near zero,

$$\begin{aligned} B(x + s\omega, \omega, E) &= (x + s\omega) - t(x + s\omega, \omega)\omega \\ &= (x + s\omega) - (t(x, \omega) + s)\omega = x - t(x, \omega)\omega \\ &= B(x, \omega, E), \end{aligned}$$

and hence

$$\begin{aligned} \omega \cdot \nabla_x (g(B(x, \omega, E), \omega, E)) &= \frac{d}{ds} \Big|_{s=0} g(B(x + s\omega, \omega, E), \omega, E) \\ &= \frac{d}{ds} \Big|_{s=0} g(B(x, \omega, E), \omega, E) \\ &= 0. \end{aligned}$$

Thus,

$$\begin{aligned} & \omega \cdot \nabla_x \psi(x, \omega, E) \\ &= \psi(x, \omega, E) \left(-\Sigma(x - t(x, \omega)\omega, \omega, E) + \Sigma(x - t(x, \omega)\omega, \omega, E) - \Sigma(x, \omega, E) \right) \\ & \quad + e^{-\int_0^{t(x, \omega)} \Sigma(x - s\omega, \omega, E) ds} \omega \cdot \nabla_x (g(B(x, \omega, E), \omega, E)) \\ &= -\Sigma(x, \omega, E) \psi(x, \omega, E), \end{aligned}$$

which is (41).

On the other hand, if $(y, \omega, E) \in \Gamma_-$, then $t(y, \omega) = 0$ by Proposition 3.7, and hence $B(y, \omega, E) = y$, which gives $\psi(y, \omega, E) = g(y, \omega, E)$ i.e. (40). \square

With the assumptions of Theorems 3.12 and 3.13 the (classical) solution of the problem

$$(43) \quad \omega \cdot \nabla \psi + \Sigma(x, \omega, E)\psi = f(x, \omega, E) \text{ in } D$$

satisfying the inhomogeneous inflow boundary condition (40) is the sum $\psi + \phi$ of the solutions of the problems

$$(44) \quad \begin{aligned} \omega \cdot \nabla \psi + \Sigma(x, \omega, E)\psi &= f(x, \omega, E) \text{ in } D \\ \psi(y, \omega, E) &= 0 \text{ on } \Gamma_-, \end{aligned}$$

and

$$(45) \quad \begin{aligned} \omega \cdot \nabla \phi + \Sigma(x, \omega, E)\phi &= 0 \text{ in } D \\ \phi(y, \omega, E) &= g(y, \omega, E) \text{ on } \Gamma_- \end{aligned}$$

Hence we obtain under the assumptions of Theorems 3.12, 3.13 a (classical) solution ψ in D for the problem (36), (40)

$$(46) \quad \begin{aligned} \psi(x, \omega, E) &= \int_0^{t(x, \omega)} e^{\int_0^t -\Sigma(x-s\omega, \omega, E)ds} \cdot f(x-t\omega, \omega, E)dt \\ &\quad + e^{\int_0^{t(x, \omega)} -\Sigma(x-s\omega, \omega, E)ds} \cdot g(x-t(x, \omega)\omega, \omega, E). \end{aligned}$$

For later needs we also formulate a generalization of Theorem 3.13:

Suppose that $g_j \in C(\Gamma_-)$ such that $\frac{\partial g}{\partial y_i} \in C(\Gamma_-)$, $i = 1, 2$ (in the same sense as in Theorem 3.13 above) and $\Sigma_{lk} \in C(\overline{G} \times S \times I)$ such that $\frac{\partial \Sigma_{lk}}{\partial x_j} \in C(\overline{G} \times S \times I)$, $1 \leq l, k \leq 3$. Let

$$\Sigma \psi = \overline{\Sigma} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix}$$

where $\overline{\Sigma}$ is the matrix $(\Sigma_{lk}(x, \omega, E))$. Then the unique classical solution $\psi = (\psi_1, \psi_2, \psi_3)$ of the coupled system of equations

$$(47) \quad \omega \cdot \nabla \psi_j + \Sigma(x, \omega, E)\psi = 0 \text{ in } D, \quad j = 1, 2, 3$$

satisfying the inhomogeneous inflow boundary condition

$$(48) \quad \psi_j(y, \omega, E) = g_j(y, \omega, E) \text{ on } \Gamma_-, \quad j = 1, 2, 3$$

is

$$(49) \quad \psi(x, \omega, E) = e^{-\int_0^{t(x, \omega)} \overline{\Sigma}(x-s\omega, \omega, E)ds} \cdot g(x-t(x, \omega)\omega, \omega, E).$$

In the case where $\overline{\Sigma}$ is a diagonal matrix $\overline{\Sigma} = \text{diag}(\Sigma_1, \Sigma_2, \Sigma_3)$ the (classical) solution of (47-48) is

$$\begin{aligned} \psi(x, \omega, E) &= \left(e^{\int_0^{t(x, \omega)} -\Sigma_1(x-s\omega, \omega, E)ds} \cdot g_1(x-t(x, \omega)\omega, \omega, E), \right. \\ &\quad e^{\int_0^{t(x, \omega)} -\Sigma_2(x-s\omega, \omega, E)ds} \cdot g_2(x-t(x, \omega)\omega, \omega, E), \\ &\quad \left. e^{\int_0^{t(x, \omega)} -\Sigma_3(x-s\omega, \omega, E)ds} \cdot g_3(x-t(x, \omega)\omega, \omega, E) \right). \end{aligned}$$

In this article we need only this solution of uncoupled convection equation.

Similarly we find (a generalization of Theorem 3.12) that when $f_j \in C(\overline{G} \times S \times I)$, $j = 1, 2, 3$ such that $\frac{\partial f_j}{\partial x_k} \in C(\overline{G} \times S \times I)$, $j, k = 1, 2, 3$, the (classical) solution of the coupled system

$$\omega \cdot \nabla \psi_j + \Sigma(x, \omega, E) \psi = f_j(x, \omega, E) \text{ in } D, \quad j = 1, 2, 3$$

satisfying the homogeneous inflow boundary condition

$$\psi_j(y, \omega, E) = 0 \text{ on } \Gamma_-, \quad j = 1, 2, 3$$

is

$$(50) \quad \psi(x, \omega, E) = \int_0^{t(x, \omega)} e^{\int_0^t -\Sigma(x-s\omega, \omega, E) ds} \cdot f(x - t\omega, \omega, E) dt.$$

The (classical) solution for the general coupled system

$$\omega \cdot \nabla \psi_j + \Sigma(x, \omega, E) \psi = f_j(x, \omega, E) \text{ in } D, \quad j = 1, 2, 3$$

satisfying the inhomogeneous inflow boundary condition

$$\psi_j(y, \omega, E) = g_j(y, \omega, E) \text{ on } \Gamma_-, \quad j = 1, 2, 3$$

is obtained as the sum of solutions (49) and (50) (when the stated assumptions are valid).

Remark 3.14 The classical solution ψ obtained above is continuous in D (and its partial derivatives $\frac{\partial \psi}{\partial x_k}$, $k = 1, 2, 3$ are continuous in D) which can be immediately seen from the formulas like (31) and (42). Thus ψ is continuous almost everywhere in $G \times S \times I$, which implies in particular that it is Lebesgue measurable in $G \times S \times I$.

Note that in the case where G is convex such that ∂G is C^1 -boundary, the solution ψ is in $C(\overline{G} \times S \times I)$ and $\frac{\partial \psi}{\partial x_k} \in C(G \times S \times I)$.

Remark 3.15 Notice that the formulas for ψ in Theorems 3.12 and 3.13 make sense under the less restrictive assumptions $f \in C(\overline{G} \times S \times I)$ and $g \in C(\Gamma_-)$, respectively, i.e. assuming that f and g are merely continuous (and $\Sigma \in C(\overline{G} \times S \times I)$), but not necessarily continuously differentiable with respect to x and y , respectively. Then these ψ s can be considered as generalized (classical) solutions to the corresponding boundary value problems in the sense that if, by convention, we replace $\omega \cdot \nabla \psi$ by $\frac{d}{ds} \psi(x + s\omega, \omega, E)|_{s=0}$, then (36)-(37) and (39)-(40) are satisfied for all $(x, \omega, E) \in D$.

4. DISSIPATIVITY OF THE CONVECTION OPERATOR

4.1. On Dissipativity of Linear Operators in Banach Spaces. Let X be a real Banach space and let X^* be its dual space. Suppose that $x \in X$. Denote by $J(x) = J_X(x)$ the subset of X^* defined by

$$J(x) = \{l \in X^* \mid \|l\|_{X^*} = \|x\|_X \text{ and } \langle l, x \rangle := l(x) = \|x\|_X \|l\|_{X^*}\}.$$

In the product space $X = X_1 \times X_2 \times X_3$ we use the norm

$$\|x\|_{X_1 \times X_2 \times X_3} = \sum_{j=1}^3 \|x_j\|_{X_j}, \quad x = (x_1, x_2, x_3) \in X.$$

One has that $X^* = X_1^* \oplus X_2^* \oplus X_3^*$ in the sense that for any $l \in X^*$,

$$l(x) = \sum_{j=1}^3 \langle l_j, x_j \rangle,$$

where $l_j := l|_{X_j} \in X_j^*$, and the corresponding norm is given by $\|l\|_{X^*} = \max_{1 \leq j \leq 3} \|l_j\|_{X_j^*}$. The structure of $J_X(x)$ can be obtained by applying iteratively the following lemma.

Lemma 4.1 Let Y_1, Y_2 be Banach spaces, $Y = Y_1 \oplus Y_2$ their product equipped with the 1-norm $\|y\|_Y = \|y_1\|_{Y_1} + \|y_2\|_{Y_2}$, $y = (y_1, y_2) \in Y$ like above. Then for every $y = (y_1, y_2) \in Y$ we have

$$(51) \quad J_Y(y) = \begin{cases} J_{Y_1}(z_1(y)) \times J_{Y_2}(z_2(y)), & \text{if } y_1 \neq 0 \text{ and } y_2 \neq 0, \\ \overline{B}_{Y_1^*}(\|y_2\|_{Y_2}) \times J_{Y_2}(y_2), & \text{if } y_1 = 0, \\ J_{Y_1}(y_1) \times \overline{B}_{Y_2^*}(\|y_1\|_{Y_1}), & \text{if } y_2 = 0, \end{cases}$$

where $\overline{B}_{Y_j^*}(r)$ denotes the closed ball of radius $r > 0$ in Y_j^* ,

$$z_j(y) := \frac{\|y\|_Y}{\|y_j\|_{Y_j}} y_j, \quad \text{when } y_j \neq 0, \quad j = 1, 2.$$

Proof. Let $l \in J_Y(y)$. Then by the definition of J_Y

$$(52) \quad \begin{aligned} \|l\|_{Y^*} &= \|y\|_Y = \|y_1\|_{Y_1} + \|y_2\|_{Y_2} \\ (\|y_1\|_{Y_1} + \|y_2\|_{Y_2}) \|l\|_{Y^*} &= \|y\|_Y \|l\|_{Y^*} = l(y) = l_1(y_1) + l_2(y_2). \end{aligned}$$

Recalling that $\|l\|_{Y^*} = \max\{\|l_1\|_{Y_1^*}, \|l_2\|_{Y_2^*}\}$, the second line above implies that

$$\begin{aligned} (\|y_1\|_{Y_1} + \|y_2\|_{Y_2}) \|l\|_{Y^*} &= l_1(y_1) + l_2(y_2) \leq \|l_1\|_{Y_1^*} \|y_1\|_{Y_1} + \|l_2\|_{Y_2^*} \|y_2\|_{Y_2} \\ &\leq \|l\|_{Y^*} (\|y_1\|_{Y_1} + \|y_2\|_{Y_2}), \end{aligned}$$

i.e.

$$(\|y_1\|_{Y_1} + \|y_2\|_{Y_2}) \|l\|_{Y^*} = l_1(y_1) + l_2(y_2) = \|l_1\|_{Y_1^*} \|y_1\|_{Y_1} + \|l_2\|_{Y_2^*} \|y_2\|_{Y_2}.$$

Taking into account the fact that $\|l\|_{Y^*} \geq \|l_1\|_{Y_1^*}, \|l_2\|_{Y_2^*}$, one can conclude from the above equality that

$$(53) \quad \begin{aligned} l_1(y_1) &= \|y_1\|_{Y_1} \|l_1\|_{Y_1^*} = \|y_1\|_{Y_1} \|l\|_{Y^*} \\ l_2(y_2) &= \|y_2\|_{Y_2} \|l_2\|_{Y_2^*} = \|y_2\|_{Y_2} \|l\|_{Y^*}. \end{aligned}$$

Assume first that $y_1 = 0$. If $y_2 = 0$ as well, we have $\|l\|_{Y^*} = 0$ from the first line of (52) and thus $\|l_1\|_{Y_1^*} = \|l_2\|_{Y_2^*} = 0$, which means that $(l_1, l_2) = (0, 0) \in \overline{B}_{Y_1^*}(\|y_2\|_{Y_2}) \times J_{Y_2}(y_2)$. On the other hand, if $y_2 \neq 0$, the second line of (53) implies that $\|l\|_{Y^*} = \|l_2\|_{Y_2^*}$, and hence from (52), we have $\|l_2\|_{Y_2^*} = \|y_2\|_{Y_2}$. Because $\|l_1\|_{Y_1^*} \leq \|l\|_{Y^*} = \|y_2\|_{Y_2}$, this shows that $(l_1, l_2) \in \overline{B}_{Y_1^*}(\|y_2\|_{Y_2}) \times J_{Y_2}(y_2)$.

The case where $y_2 = 0$ and y_1 is arbitrary is handled similarly.

We may thus assume that both y_1 and y_2 are non-zero. Using (53) and the definition of $z_j(y)$ as given above, one has

$$l_j(z_j(y)) = \frac{\|y\|_Y}{\|y_j\|_{Y_j}} l_j(y_1) = \|y\|_Y \|l_j\|_{Y_j^*} = \|z_j(y)\|_{Y_j} \|l_j\|_{Y_j^*}, \quad j = 1, 2.$$

On the other hand, (53) implies that $\|l\|_{Y^*} = \|l_1\|_{Y_1^*} = \|l_2\|_{Y_2^*}$, and hence by using (52),

$$\|z_j(y)\|_{Y_j} = \|y\|_Y = \|l\|_{Y^*} = \|l_j\|_{Y_j^*}.$$

By the definition of the duality set, then, we conclude that $l_j \in J_{Y_j}(z_j(y))$, $j = 1, 2$.

We have thus shown that the set $J_Y(y)$ is a subset of the right hand side of (51), taking the appropriate cases into account. The reverse inclusion is readily verified by checking, case by case, the validity of both of the lines in (52). \square

In this section, we assume that $A : D(A) \subset X \rightarrow X$ is *densily defined*, i.e. the domain of definition $D(A)$ of A is dense in X . In addition, instead of $A : D(A) \subset X \rightarrow X$ we usually write simply $A : X \rightarrow X$.

Definition 4.2 (i) An (unbounded) linear operator $A : X \rightarrow X$ is said to be *dissipative*, if for each $x \in D(A)$ there exists $l \in J(x)$ such that

$$(54) \quad \langle l, Ax \rangle \leq 0.$$

The operator $A : X \rightarrow X$ is said to be *accretive*, if $-A$ is dissipative.

(ii) A dissipative operator $A : X \rightarrow X$ is *m-dissipative*, if there exists $\lambda > 0$ such that

$$R(\lambda I - A) = X,$$

where $R(\lambda I - A)$ is the range of $\lambda I - A$ and I is the identity operator.

One knows that if an operator $A : X \rightarrow X$ is dissipative and if there exists $\lambda_0 > 0$ such that $R(\lambda_0 I - A) = X$ then $R(\lambda I - A) = X$ for every $\lambda > 0$ ([42], Section 1.4, [21], Section II.3.b). On the other hand, the condition $R(\lambda I - A) = X$ is equivalent to $\lambda \in \rho(A)$ (the resolvent set of A) in the case when A is dissipative, as follows from the theorem we present next.

Theorem 4.3 A linear operator $A : X \rightarrow X$ is dissipative if and only if for all $\lambda > 0$ the estimate

$$(55) \quad \|(\lambda I - A)x\| \geq \lambda \|x\|, \quad \forall x \in D(A),$$

holds.

Proof. For the proof we refer to [21], Section II.3.b or [42], Section 1.4. \square

In particular, *m*-dissipative operator A is closed since $\rho(A) \neq \emptyset$. We also have the following (bounded) perturbation result for *m*-dissipative operators.

Theorem 4.4 Suppose that a closed operator $A : X \rightarrow X$ is *m*-dissipative and that $B : X \rightarrow X$ is a bounded dissipative operator. Then $A + B : X \rightarrow X$ is *m*-dissipative.

Proof. See [42] (Chap. 1, Theorem 4.3 and Chap. 3, Corollary 3.3) or [21] (Chap. II, Theorem 3.15 and Chap. III, Theorem 2.7).

Here is a sketch of the proof. Given $x \in D(A)$, since B is dissipative and bounded ($D(B) = X$), there exists $l \in J(x)$, such that $\langle l, Bx \rangle \leq 0$. But because A is *m*-dissipative, one also has $\langle l, Ax \rangle \leq 0$ ([42], Theorem 4.3 (b)), and hence

$$\langle l, (A + B)x \rangle \leq 0,$$

which shows that $A + B$ is dissipative.

It remains to show that $\lambda I - (A + B)$ is surjective for some $\lambda > 0$. Taking $\lambda > \|B\|$, the *m*-dissipativity of A implies that $\lambda \in \rho(A)$ and

$$\|(\lambda I - A)^{-1}B\| \leq \frac{\|B\|}{\lambda} < 1,$$

which shows that $I - (\lambda I - A)^{-1}B$ has a bounded inverse. On the other hand,

$$\lambda I - (A + B) = (\lambda I - A)(I - (\lambda I - A)^{-1}B),$$

which shows that $\lambda I - (A + B)$ has a bounded inverse. In particular, $\lambda I - (A + B)$ is surjective and the proof is complete. \square

In the case where $X = L^1(G \times S \times I)$ we have $L^1(G \times S \times I)^* = L^\infty(G \times S \times I)$ isomorphically (and isometrically) and for $l \in L^1(G \times S \times I)^*$ and $\psi \in L^1(G \times S \times I)$ one has (recall that we have everywhere real spaces)

$$l(\psi) = \langle w, \psi \rangle = \int_{G \times S \times I} w \psi dx d\omega dE$$

where $w \in L^1(G \times S \times I)^\infty$ is corresponding to $l \in L^1(G \times S \times I)^*$ through the above mentioned isomorphism.

It is well known that that for $\psi \in L^1(G \times S \times I)$

$$J(\psi) = \{w \in L^\infty(G \times S \times I) \mid w = \|\psi\|_{L^1(G \times S \times I)} \psi^*\}$$

(cf. [18] Chapter XVII, section 3.2, p. 344, or use Theorem 1.40 in [45]) where

$$\psi^*(x, \omega, E) = \begin{cases} 1, & \psi(x, \omega, E) > 0 \\ -1, & \psi(x, \omega, E) < 0 \end{cases}$$

and ψ^* is a measurable function for which $|\psi^*(x, \omega, E)| \leq 1$ when $\psi(x, \omega, E) = 0$. As defined above a linear operator $A : L^1(G \times S \times I) \rightarrow L^1(G \times S \times I)$ is dissipative, if for each $\psi \in D(A)$ there exists $w \in J(\psi)$ such that

$$(56) \quad \langle w, A\psi \rangle = \int_{G \times S \times I} w A\psi dx d\omega dE \leq 0.$$

Assume that $\psi \neq 0$. We choose $\psi^*(x, \omega, E) = 0$ when $\psi(x, \omega, E) = 0$. Then the condition (56) (for that w) means that (here $\text{sign}(\psi)$ is the signum function)

$$(57) \quad \int_{G \times S \times I} \|\psi\|_{L^1(G \times S \times I)} \psi^* A\psi dx d\omega dE = \|\psi\|_{L^1(G \times S \times I)} \int_{G \times S \times I} \text{sign}(\psi) A\psi dx d\omega dE \leq 0$$

that is

$$(58) \quad \int_{G \times S \times I} \text{sign}(\psi) A\psi dx d\omega dE \leq 0.$$

4.2. m -dissipativity of the Convection Operator. Let

$$\tilde{W}_{-,0}^1(G \times S \times I) = \{\psi \in \tilde{W}^1(G \times S \times I) \mid \psi|_{\Gamma_-} = \gamma_-(\psi) = 0\}.$$

Furthermore, let $A : L^1(G \times S \times I) \rightarrow L^1(G \times S \times I)$ and $A_0 : L^1(G \times S \times I) \rightarrow L^1(G \times S \times I)$ be linear operators defined by

$$D(A) = W^1(G \times S \times I), \quad A\psi = -\omega \cdot \nabla \psi.$$

and

$$D(A_0) = \tilde{W}_{-,0}^1(G \times S \times I), \quad A_0\psi = -\omega \cdot \nabla \psi.$$

Thus the domain of A_0 (so called *realization*) consists of those $\psi \in \tilde{W}^1(G \times S \times I)$ for which $\psi|_{\Gamma_-} = \gamma_-(\psi) = 0$.

Proposition 4.5 The linear operator A_0 is closed and densely defined.

Proof. The domain $D(A_0)$ is dense in $L^1(G \times S \times I)$ since $C_0^1(G \times S \times I)$ is dense in $L^1(G \times S \times I)$.

That A_0 is closed can be seen as follows. Let $f, \psi \in L^1(G \times S \times I)$ and let $\{\psi_n\} \subset D(A_0) = \tilde{W}_{-,0}^1(G \times S \times I)$ be such that $\|\psi_n - \psi\|_{L^1(G \times S \times I)} \rightarrow 0$ and $\|A_0\psi_n - f\|_{L^1(G \times S \times I)} \rightarrow 0$ as $n \rightarrow \infty$. Then $\{\psi_n\} \subset \tilde{W}^1(G \times S \times I)$ is a Cauchy sequence in $W^1(G \times S \times I)$ and hence there exists an element $\psi' \in W^1(G \times S \times I)$ such that $\psi_n \rightarrow \psi'$ in $W^1(G \times S \times I)$. As the latter space is continuously embedded in $L^1(G \times S \times I)$, we have $\psi_n \rightarrow \psi$ also in $L^1(G \times S \times I)$, therefore $\psi = \psi'$ and so $\psi_n \rightarrow \psi$ in $W^1(G \times S \times I)$. Because the trace mapping $\gamma_- : W^1(G \times S \times I) \rightarrow L_{\text{loc}}^1(\Gamma_-, |\omega \cdot \nu| d\sigma d\omega dE)$ is continuous we get that $\gamma_-(\psi_n) \rightarrow \gamma_-(\psi)$ in $L_{\text{loc}}^1(\Gamma_-, |\omega \cdot \nu| d\sigma d\omega dE)$ and since $\gamma_-(\psi_n) = 0$, also $\gamma_-(\psi) = 0$. Hence $\psi \in \tilde{W}_{-,0}^1(G \times S \times I) = D(A_0)$ and $A_0\psi = -\omega \cdot \nabla \psi = \lim_{n \rightarrow \infty} -\omega \cdot \nabla \psi_n = f$, which shows that A_0 is closed. \square

Lemma 4.6 Let $f \in C(\overline{G} \times S \times I)$ such that $\frac{\partial f}{\partial x_j} \in C(\overline{G} \times S \times I)$ for $j = 1, 2, 3$. Then the (classical) solution (cf. Theorem 3.11) $\psi : G \times S \times I \rightarrow \mathbb{R}$ of the equation ($\lambda \in \mathbb{R}$)

$$\omega \cdot \nabla \psi + \lambda \psi = f(x, \omega, E) \quad \Longleftrightarrow \quad (\lambda I - A)\psi = f$$

defined by $\psi(x, \omega, E) = \int_0^{t(x, \omega)} e^{-\lambda t} f(x - t\omega, \omega, E) dt$ belongs to $\tilde{W}_{-,0}^1(G \times S \times I) = D(A_0)$. In addition for any $\lambda > 0$

$$(59) \quad \|\psi\|_{L^1(G \times S \times I)} \leq \frac{1}{\lambda} \|f\|_{L^1(G \times S \times I)} = \frac{1}{\lambda} \|(\lambda I - A_0)\psi\|_{L^1(G \times S \times I)}.$$

Proof. Due to Remark 3.14 ψ is measurable in $G \times S \times I$. We show that $\psi \in W^1(G \times S \times I)$. Since $\omega \cdot \nabla \psi + \lambda \psi = f \in C(\overline{G} \times S \times I) \subset L^1(G \times S \times I)$ it suffices to verify that $\psi \in L^1(G \times S \times I)$. Denoting by \bar{f} the extension by zero of f on $\mathbb{R}^3 \times S \times I$, we have

$$(60) \quad \psi(x, \omega, E) = \int_0^\infty e^{-\lambda t} \bar{f}(x - t\omega, \omega, E) \chi_{[0, t(x, \omega)]}(t) dt$$

where $\chi_{[0, t(x, \omega)]}$ is the characteristic function of the interval $[0, t(x, \omega)]$ (note that the integrand of (60) is measurable).

Hence applying the change of variables $x - t\omega = z$ (in x -variable) we obtain

$$(61) \quad \begin{aligned} \|\psi\|_{L^1(G \times S \times I)} &= \int_{G \times S \times I} |\psi(x, \omega, E)| dx d\omega dE \\ &\leq \int_0^\infty e^{-\lambda t} \int_G \int_{S \times I} |\bar{f}(x - t\omega, \omega, E)| \chi_{[0, t(x, \omega)]}(t) dx d\omega dE dt \\ &= \int_0^\infty e^{-\lambda t} \int_{S \times I} \int_{(G - t\omega) \cap G} |\bar{f}(z, \omega, E)| \chi_{[0, t(z + t\omega, \omega)]}(t) dz d\omega dE dt \\ &\leq \int_0^\infty e^{-\lambda t} \int_G \int_{S \times I} |f(z, \omega, E)| dz d\omega dE dt = \frac{1}{\lambda} \|f\|_{L^1(G \times S \times I)}. \end{aligned}$$

Hence $\psi \in L^1(G \times S \times I)$ and the estimate (59) holds.

By Theorem 3.11 the inflow boundary condition $\psi(y, \omega, E) = 0$ is true a.e. $(y, \omega, E) \in \Gamma_-$ (in the classical sense). Hence the proof is complete. \square

The following theorem is shown by different methods in [19], section XXI.§2, Theorem 2 and Remark 3 (pp. 222-224). An alternative proof is also given in section XXI.§2, Prop. 5 (pp. 242-243) in [19].

Theorem 4.7 The operator $A_0 : L^1(G \times S \times I) \rightarrow L^1(G \times S \times I)$ is m -dissipative.

Proof. A. We show that $R(\lambda I - A_0) = L^1(G \times S \times I)$ for any $\lambda > 0$. Let $f \in L^1(G \times S \times I)$. Then there exists a sequence $\{f_n\} \subset \mathcal{D}(\overline{G} \times S \times I)$ such that $\|f_n - f\|_{L^1(G \times S \times I)} \rightarrow 0$ when $n \rightarrow \infty$. By Lemma 4.6 there exists $\psi_n \in D(A_0) = \tilde{W}_{-,0}^1(G \times S \times I)$ such that $(\lambda I - A_0)\psi_n = f_n$ and

(62)

$$\|\psi_n - \psi_m\|_{L^1(G \times S \times I)} \leq \frac{1}{\lambda} \|(\lambda I - A_0)(\psi_n - \psi_m)\|_{L^1(G \times S \times I)} = \frac{1}{\lambda} \|f_n - f_m\|_{L^1(G \times S \times I)}$$

which implies that $\psi_n \rightarrow \psi$ in $L^1(G \times S \times I)$ for some $\psi \in L^1(G \times S \times I)$. Since also $(\lambda I - A_0)\psi_n = f_n \rightarrow f$ in $L^1(G \times S \times I)$ and since $\lambda I - A_0$ is closed we obtain that $\psi \in D(A_0)$ and $(\lambda I - A_0)\psi = f$.

B. Since by Lemma 4.6 again, for all $n \in \mathbb{N}$ and $\lambda > 0$ the estimate

$$\|(\lambda I - A_0)\psi_n\| \geq \lambda \|\psi_n\|$$

is valid we see that

$$(63) \quad \|(\lambda I - A_0)\psi\| \geq \lambda \|\psi\| \text{ for all } \psi \in D(A_0).$$

Due to Theorem 4.3 A_0 is dissipative and hence by Part A of the proof A_0 is m -dissipative. This completes the proof.

Remark 4.8 An alternative proof for the dissipativity of A_0 can be seen by applying the Green formula (see e.g. [19], pp. 242-243) as follows. One knows that $|\psi| \in W^1(G \times S \times I)$ when $\psi \in W^1(G \times S \times I)$ and (cf. [27], Sections 5.1–5.2)

$$(64) \quad \omega \cdot \nabla(|\psi|) = \text{sign}(\psi)\omega \cdot \nabla\psi$$

in $W^1(G \times S \times I)$. Applying (9) for $u = |\psi|$ then gives

$$\begin{aligned} & - \int_{G \times S \times I} \text{sign}(\psi) A_0 \psi dx d\omega dE = \int_{G \times S \times I} \omega \cdot \nabla(|\psi|) dx d\omega dE \\ & = \int_{\partial G \times S \times I} (\omega \cdot \nu) |\psi| d\sigma d\omega dE = \int_{\Gamma_+} (\omega \cdot \nu) |\psi| d\sigma d\omega dE \geq 0, \end{aligned}$$

since $\int_{\Gamma_-} (\omega \cdot \nu(y)) |\psi| d\sigma d\omega dE = 0$ (recall that $\psi = 0$ on Γ_-), $\nabla v = 0$ and $\omega \cdot \nu(y) > 0$ on Γ_+ . Hence (58) holds, and so A_0 is dissipative for the reasons explained at the end of the corresponding section 4.1.

Lemma 4.6 and the proof of the above theorem imply that for $\lambda > 0$ the solution $\psi \in D(A_0)$ of the equation

$$(\lambda I - A_0)\psi = f, \quad f \in L^1(G \times S \times I),$$

is given by

(65)

$$\psi = \lim_{n \rightarrow \infty} \psi_n = \lim_{n \rightarrow \infty} \left(\int_0^{t(x,\omega)} f_n(x - t\omega, \omega, E) e^{-\lambda t} dt \right) = \int_0^{t(x,\omega)} f(x - t\omega, \omega, E) e^{-\lambda t} dt,$$

almost everywhere on $G \times S \times I$. Hence for $\lambda > 0$ the resolvent $(\lambda I - A_0)^{-1} : L^1(G \times S \times I) \rightarrow L^1(G \times S \times I)$ is given explicitly by

$$(66) \quad (\lambda I - A_0)^{-1} f = \int_0^{t(x, \omega)} f(x - t\omega, \omega, E) e^{-\lambda t} dt$$

and the resolvent satisfies the estimate

$$\|(\lambda I - A_0)^{-1} f\|_{L^1(G \times S \times I)} \leq \frac{1}{\lambda} \|f\|_{L^1(G \times S \times I)}, \quad \lambda > 0.$$

5. COUPLED BOLTZMANN TRANSPORT EQUATION

5.1. m -dissipativity of Cartesian Product Convection Operator. As we mentioned above in Section 4.1 in the Cartesian product space $L^1(G \times S \times I)^3$ we use the norm

$$\|\psi\|_{L^1(G \times S \times I)^3} = \sum_{j=1}^3 \|\psi_j\|_{L^1(G \times S \times I)}, \quad \psi = (\psi_1, \psi_2, \psi_3).$$

and similarly in its subspaces $X^3 \subset L^1(G \times S \times I)^3$, $X \subset L^1(G \times S \times I)$ we use the norms

$$\|\psi\|_{X^3} = \sum_{j=1}^3 \|\psi_j\|_X, \quad \psi = (\psi_1, \psi_2, \psi_3).$$

Define linear operators \mathbf{A} and $\mathbf{A}_0 : L^1(G \times S \times I)^3 \rightarrow L^1(G \times S \times I)^3$ by

$$\begin{aligned} D(\mathbf{A}) &= W^1(G \times S \times I)^3 \\ \mathbf{A}\psi &= (-\omega \cdot \nabla \psi_1, -\omega \cdot \nabla \psi_2, -\omega \cdot \nabla \psi_3). \end{aligned}$$

and

$$D(\mathbf{A}_0) = W_{-,0}^1(G \times S \times I)^3, \quad \mathbf{A}_0\psi = \mathbf{A}\psi.$$

We see that

$$\mathbf{A}\psi = \begin{pmatrix} A & 0 & 0 \\ 0 & A & 0 \\ 0 & 0 & A \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix}$$

where $A : L^1(G \times S \times I) \rightarrow L^1(G \times S \times I)$ is above in Section 4 defined operator and similarly for \mathbf{A}_0 .

Since A_0 (whose domain is $D(A_0) = W_{-,0}^1(G \times S \times I)$) is a closed densely defined operator we see that $\mathbf{A}_0 : L^1(G \times S \times I)^3 \rightarrow L^1(G \times S \times I)^3$ is a closed densely defined operator.

Theorem 5.1 The operator $\mathbf{A}_0 : L^1(G \times S \times I)^3 \rightarrow L^1(G \times S \times I)^3$ is m -dissipative.

Proof. We find by (63) that for all $\psi \in D(\mathbf{A}_0)$ and $\lambda > 0$

$$\begin{aligned} \|(\lambda I - \mathbf{A}_0)\psi\|_{L^1(G \times S \times I)^3} &= \sum_{j=1}^3 \|(\lambda I - A_0)\psi_j\|_{L^1(G \times S \times I)} \\ &\geq \lambda \sum_{j=1}^3 \|\psi_j\|_{L^1(G \times S \times I)} = \lambda \|\psi\|_{L^1(G \times S \times I)^3} \end{aligned}$$

and then \mathbf{A}_0 is dissipative by Theorem 4.3.

We verify that \mathbf{A}_0 is m -dissipative that is, in addition to dissipativity one has $R(\lambda I - \mathbf{A}_0) = L^1(G \times S \times I)^3$ for (any) $\lambda > 0$. Let $f = (f_1, f_2, f_3) \in L^1(G \times S \times I)^3$. Then by Theorem 4.7 for any $j = 1, 2, 3$ there exists $\psi_j \in D(A_0) = \tilde{W}_{-,0}^1(G \times S \times I)$ such that $(\lambda I - A_0)\psi_j = f_j$ and so $R(\lambda I - \mathbf{A}_0) = L^1(G \times S \times I)^3$ for any $\lambda > 0$. This completes the proof. \square

5.2. Dissipativity of Scattering-Collision Operator. Let $\Sigma_j : G \times S \times I \rightarrow \mathbb{R}$, $j = 1, 2, 3$ be functions, the so-called *total cross sections*, such that

$$(67) \quad \Sigma_j \in L^\infty(G \times S \times I), \quad \Sigma_j \geq 0 \text{ a.e. in } G \times S \times I, \quad j = 1, 2, 3.$$

Furthermore, let $\sigma_{kj} : G \times S^2 \times I^2 \rightarrow \mathbb{R}$, $1 \leq k, j \leq 3$ be measurable functions, the so-called *differential cross sections*, such that

$$(68) \quad \sum_{k=1}^3 \int_{S \times I} \sigma_{jk}(x, \omega, \omega', E, E') d\omega' dE' \leq C \text{ a.e. } (x, \omega, E) \in G \times S \times I, \\ \sigma_{kj} \geq 0 \text{ a.e. in } G \times S^2 \times I^2, \quad k, j = 1, 2, 3$$

and

$$(69) \quad \sum_{k=1}^3 \int_{S \times I} \sigma_{kj}(x, \omega, \omega', E, E') d\omega' dE' \leq C \text{ a.e. } (x, \omega, E) \in G \times S \times I, \quad j = 1, 2, 3.$$

In the case $p = 1$ we will only need the condition (68).

Define the *scattering operator* Σ_j and the *collision operator* K_j corresponding to the particle j for $j = 1, 2, 3$ as follows

$$(70) \quad (\Sigma_j \psi_j)(x, \omega, E) = \Sigma_j(x, \omega, E) \psi_j(x, \omega, E), \quad \psi_j \in L^1(G \times S \times I)$$

and

$$(71) \quad (K_j \psi)(x, \omega, E) = \sum_{k=1}^3 \int_{S \times I} \sigma_{kj}(x, \omega', \omega, E', E) \psi_k(x, \omega', E') d\omega' dE',$$

where $\psi \in L^1(G \times S \times I)^3$. Furthermore, we define for $\psi \in L^1(G \times S \times I)^3$

$$(72) \quad \Sigma \psi = (\Sigma_1 \psi_1, \Sigma_2 \psi_2, \Sigma_3 \psi_3)$$

and

$$(73) \quad K \psi = (K_1 \psi, K_2 \psi, K_3 \psi).$$

The operators Σ and K are linear and continuous, as we formulate next.

Theorem 5.2 The operators Σ and K are bounded linear maps $L^1(G \times S \times I)^3 \rightarrow L^1(G \times S \times I)^3$.

Proof. We see that

$$\begin{aligned} \|\Sigma_j \psi_j\|_{L^1(G \times S \times I)} &= \int_{G \times S \times I} |\Sigma_j(x, \omega, E) \psi_j(x, \omega, E)| dx d\omega dE \\ &\leq \|\Sigma_j\|_{L^\infty(G \times S \times I)} \|\psi_j\|_{L^1(G \times S \times I)} \end{aligned}$$

and then

$$(74) \quad \|\Sigma \psi\|_{L^1(G \times S \times I)^3} \leq \max_{1 \leq j \leq 3} \|\Sigma_j\|_{L^\infty(G \times S \times I)} \|\psi\|_{L^1(G \times S \times I)^3}.$$

Furthermore,

$$\begin{aligned}
\|K_j\psi\|_{L^1(G \times S \times I)} &= \int_{G \times S \times I} \left| \left(\sum_{k=1}^3 \int_{S \times I} \sigma_{kj}(x, \omega', \omega, E', E) \psi_k(x, \omega', E') d\omega' dE' \right) \right| dx d\omega dE \\
(75) \quad &\leq \int_G \left(\int_{S \times I} \left(\sum_{k=1}^3 \int_{S \times I} \sigma_{kj}(x, \omega', \omega, E', E) d\omega dE \right) |\psi_k(x, \omega', E')| d\omega' dE' \right) dx,
\end{aligned}$$

and then by the assumption (68)

$$(76) \quad \|K\psi\|_{L^1(G \times S \times I)^3} \leq C \sum_{k=1}^3 \int_G \int_{S \times I} |\psi_k(x, \omega', E')| d\omega' dE' dx = C \|\psi\|_{L^1(G \times S \times I)^3}.$$

The assertion follows from (74) and (76). \square

In order that the operator $-(\Sigma - K) = -\Sigma + K : L^1(G \times S \times I)^3 \rightarrow L^1(G \times S \times I)^3$ would be dissipative we assume that the cross-sections satisfy the following condition:

There exists $c \geq 0$ such that for every $j = 1, 2, 3$ (cf. [19], pp. 241 for one particle and [51], [9] for coupled system)

$$(77) \quad \Sigma_j(x, \omega, E) - \sum_{k=1}^3 \int_{S \times I} \sigma_{jk}(x, \omega, \omega', E, E') d\omega' dE' \geq c, \text{ a.e. } (x, \omega, E) \in G \times S \times I.$$

and

$$(78) \quad \Sigma_j(x, \omega, E) - \sum_{k=1}^3 \int_{S \times I} \sigma_{kj}(x, \omega', \omega, E', E) d\omega' dE' \geq c, \text{ a.e. } (x, \omega, E) \in G \times S \times I.$$

When considering L^1 -solutions we need only the assumption (77).

We show next the following dissipativity type result for $-\Sigma + K$.

Theorem 5.3 Suppose that the assumptions (67), (68) and (77) are valid for some constant $c > 0$. Then the operator $-\Sigma + K$ satisfies the following dissipativity condition: For all $\lambda > 0$ and $\psi \in L^1(G \times S \times I)^3$ one has

$$(79) \quad \|(\lambda I - (-\Sigma + K + cI))\psi\|_{L^1(G \times S \times I)^3} \geq \lambda \|\psi\|_{L^1(G \times S \times I)^3}.$$

In other words, the operator $-\Sigma + K + cI : L^1(G \times S \times I)^3 \rightarrow L^1(G \times S \times I)^3$ is dissipative.

Proof. We have for any $\psi \in L^1(G \times S \times I)^3$ and $\lambda > 0$,

$$\begin{aligned}
\|(\lambda I - (-\Sigma + K + cI))\psi\|_{L^1(G \times S \times I)^3} &= \sum_{j=1}^3 \|(\lambda I - cI + \Sigma_j)\psi_j - K_j\psi\|_{L^1(G \times S \times I)} \\
&= \sum_{j=1}^3 \int_{G \times S \times I} \left| (\lambda - c + \Sigma_j(x, \omega, E))\psi_j(x, \omega, E) - (K_j\psi)(x, \omega, E) \right| dx d\omega dE \\
(80) \quad &\geq \sum_{j=1}^3 \int_{G \times S \times I} \left(|\lambda - c + \Sigma_j(x, \omega, E)| |\psi_j(x, \omega, E)| - |(K_j\psi)(x, \omega, E)| \right) dx d\omega dE.
\end{aligned}$$

Furthermore, we have

$$|(K_j\psi)(x, \omega, E)| \leq \sum_{k=1}^3 \int_{S \times I} \sigma_{kj}(x, \omega', \omega, E', E) |\psi_k(x, \omega', E')| d\omega' dE',$$

and by the assumption (77)

$$\lambda - c + \Sigma_j(x, \omega, E) \geq \lambda + \sum_{k=1}^3 \int_{S \times I} \sigma_{jk}(x, \omega, \omega', E, E') d\omega' dE' > 0,$$

which, when combined with (80), give

$$\begin{aligned} & \|(\lambda I - (-\Sigma + K + cI))\psi\|_{L^1(G \times S \times I)^3} \\ & \geq \sum_{j=1}^3 \int_G \left[\int_{S \times I} \left(\lambda + \sum_{k=1}^3 \int_{S \times I} \sigma_{jk}(x, \omega, \omega', E, E') d\omega' dE' \right) |\psi_j(x, \omega, E)| d\omega dE \right. \\ & \quad \left. - \int_{S \times I} \left(\sum_{k=1}^3 \int_{S \times I} \sigma_{kj}(x, \omega', \omega, E', E) |\psi_k(x, \omega', E')| d\omega' dE' \right) d\omega dE \right] dx \\ (81) \quad & = \lambda \|\psi\|_{L^1(G \times S \times I)^3} \\ & \quad + \int_G \left[\sum_{j=1}^3 \sum_{k=1}^3 \left(\int_{S \times I} \int_{S \times I} \sigma_{jk}(x, \omega, \omega', E, E') |\psi_j(x, \omega, E)| d\omega' dE' d\omega dE \right. \right. \\ & \quad \left. \left. - \int_{S \times I} \int_{S \times I} \sigma_{kj}(x, \omega', \omega, E', E) |\psi_k(x, \omega', E')| d\omega' dE' d\omega dE \right) \right] dx. \end{aligned}$$

Writing,

$$\begin{aligned} A_{jk}(x, \omega, E) &:= \int_{S \times I} \sigma_{jk}(x, \omega, \omega', E, E') d\omega' dE', \\ B_{jk}(x) &:= \int_{S \times I} A_{jk}(x, \omega, E) |\psi_j(x, \omega, E)| d\omega dE, \end{aligned}$$

we see that the last two terms on the right hand side of the above formula (81) can be written as

$$\int_G \sum_{j=1}^3 \sum_{k=1}^3 (B_{jk}(x) - B_{kj}(x)) dx = 0,$$

which allows us to conclude that

$$\|(\lambda I - (-\Sigma + K + cI))\psi\|_{L^1(G \times S \times I)^3} \geq \lambda \|\psi\|_{L^1(G \times S \times I)^3}.$$

This completes the proof. \square

Remark 5.4 Theorem 5.3 also implies (by substituting $\lambda + c$ for λ) that

$$\|(\lambda I - (-\Sigma + K))\psi\|_{L^1(G \times S \times I)^3} \geq (\lambda + c) \|\psi\|_{L^1(G \times S \times I)^3}$$

for all $\lambda > 0$. In particular, $-\Sigma + K$ is dissipative. Moreover, it is clear that the proof of the theorem remains valid if (77) is satisfied with the milder assumption $c \geq 0$.

Recall that the dual of $L^1(G \times S \times I)^3$ is

$$(L^1(G \times S \times I)^3)^* = \bigoplus_{j=1}^3 L^1(G \times S \times I)^* = \bigoplus_{j=1}^3 L^\infty(G \times S \times I) = L^\infty(G \times S \times I)^3,$$

in the sense that for any $l \in (L^1(G \times S \times I)^3)^*$ there exists a unique $w = (w_1, w_2, w_3) \in L^\infty(G \times S \times I)^3$ such that

$$(82) \quad l(\psi) = \langle w, \psi \rangle,$$

where

$$\langle w, \psi \rangle = \sum_{j=1}^3 \langle w_j, \psi_j \rangle = \sum_{j=1}^3 \int_{G \times S \times I} w_j \psi_j \, dx d\omega dE,$$

and, in the other direction, any $w \in L^\infty(G \times S \times I)^3$ defines by (82) a linear form belonging to $(L^1(G \times S \times I)^3)^*$. The norm in $L^\infty(G \times S \times I)^3$ is $\|w\|_{L^\infty(G \times S \times I)^3} = \max_{1 \leq j \leq 3} \|w_j\|_{L^\infty(G \times S \times I)}$.

The following corollary is a direct consequence of Theorems 4.3 and 5.3.

Corollary 5.5 Under the assumptions of Theorem 5.3, one has

$$\forall \psi \in L^1(G \times S \times I)^3, \quad \exists w \in J(\psi) \quad \text{s.t.} \quad \langle w, (\Sigma - K)\psi \rangle \geq c \|\psi\|_{L^1(G \times S \times I)^3}^2.$$

In Corollary 5.5 above, the structure of $J(\psi)$ is known by applying Lemma 4.1.

5.3. On Existence and Uniqueness of Solutions in L^1 -spaces for Coupled BTE-system. At first we consider the existence and uniqueness of solutions in the space $L^1(G \times S \times I)^3$ for the problem: Given $f = (f_1, f_2, f_3) \in L^1(G \times S \times I)^3$, find $\psi = (\psi_1, \psi_2, \psi_3) \in \tilde{W}_{-,0}^1(G \times S \times I)^3$ such that

$$(83) \quad \begin{aligned} \omega \cdot \nabla \psi_j + \Sigma_j \psi - K_j \psi &= f_j(x, \omega, E), \\ \psi_j|_{\Gamma_-} &= 0, \end{aligned}$$

for $j = 1, 2, 3$.

Using the notations introduced earlier, the problem (83) is equivalent to

$$(-\mathbf{A}_0 + \Sigma - K)\psi = f$$

where $f = (f_1, f_2, f_3)$ and $\psi = (\psi_1, \psi_2, \psi_3) \in D(\mathbf{A}_0) = \tilde{W}_{-,0}^1(G \times S \times I)^3$. The (unique) solvability of the problem (83) is of course equivalent to the (unique) solvability of the problem

$$(\mathbf{A}_0 - \Sigma + K)\psi = f.$$

For the rest of the section, we assume everywhere that $c > 0$ in (77).

Theorem 5.6 Suppose that the assumptions (67), (68) and (77) are valid. Then for every $f \in L^1(G \times S \times I)^3$ the problem (83) has a unique solution $\psi \in \tilde{W}_{-,0}^1(G \times S \times I)^3$.

Proof. By Theorem 5.1 the operator $\mathbf{A}_0 : L^1(G \times S \times I)^3 \rightarrow L^1(G \times S \times I)^3$ is m -dissipative and by Theorem 5.3 the operator $-(\Sigma - K) + cI : L^1(G \times S \times I)^3 \rightarrow L^1(G \times S \times I)^3$ is dissipative. Hence according to Theorem 4.4 the sum $\mathbf{A}_0 - (\Sigma - K) + cI : L^1(G \times S \times I)^3 \rightarrow L^1(G \times S \times I)$ is m -dissipative. This implies, as $c > 0$, that $R(cI - (\mathbf{A}_0 - (\Sigma - K) + cI)) = R(-\mathbf{A}_0 + \Sigma - K) = L^1(G \times S \times I)^3$, and so the existence of solutions follows.

Because $c > 0$ and since $\mathbf{A}_0 - (\Sigma - K) + cI$ is dissipative, we have by (55) of Theorem 4.3 that

$$(84) \quad \|(-\mathbf{A}_0 + \Sigma - K)\psi\|_{L^1(G \times S \times I)^3} \geq c \|\psi\|_{L^1(G \times S \times I)^3},$$

which implies the uniqueness of the solution. This completes the proof. \square

Remark 5.7 We note that the inequality (84) implies that for all $f \in L^1(G \times S \times I)^3$

$$(85) \quad \|(-\mathbf{A}_0 + \Sigma - K)^{-1}f\|_{L^1(G \times S \times I)^3} \leq \frac{1}{c} \|f\|_{L^1(G \times S \times I)^3},$$

or in other words, the solution of the problem (83) satisfies

$$(86) \quad \|\psi\|_{L^1(G \times S \times I)^3} \leq \frac{1}{c} \|f\|_{L^1(G \times S \times I)^3}.$$

For the consideration of inhomogeneous inflow boundary data we need some detailed information from the trace mapping $\gamma_- : \tilde{W}^1(G \times S \times I) \rightarrow T^1(\Gamma_-)$.

We have (cf. [19], p. 252 and [14], [15], [16])

Lemma 5.8 Every $g \in T^1(\Gamma_-)$ has an extension, called the *lift*, $\psi = Lg \in \tilde{W}^1(G \times S \times I)$ such that $\gamma_-(Lg) = (Lg)|_{\Gamma_-} = g$. In addition, the linear lift operator $L : T^1(\Gamma_-) \rightarrow \tilde{W}^1(G \times S \times I)$ satisfies

$$(87) \quad \nabla(Lg) = 0$$

and

$$(88) \quad \|Lg\|_{L^1(G \times S \times I)} = \|Lg\|_{W^1(G \times S \times I)} \leq d \|g\|_{T^1(\Gamma_-)} \text{ for all } g \in T^1(\Gamma_-)$$

where d is the diameter of G .

Proof. Let $g \in T^1(\Gamma_-)$. Define $Lg : G \times S \times I \rightarrow \mathbb{R}$ by

$$(89) \quad (Lg)(x, \omega, E) = g(x - t(x, \omega)\omega, \omega, E).$$

Using Theorem 3.13 and limiting techniques, we have that $\omega \cdot \nabla(Lg) = 0$ in $L^1(G \times S \times I)$. In addition, $\gamma_-(Lg) = g$ since $t(y, \omega) = 0$ a.e. $(y, \omega, E) \in \Gamma_-$. We have to show that $Lg \in L^1(G \times S \times I)$ and that the estimate (88) holds.

We apply the known change of variables (see e.g. [15], Prop. 2.1.). Define for $(y, \omega) \in \partial G \times S$,

$$t_+(y, \omega) = \inf\{s > 0 \mid y + s\omega \notin G\}.$$

We find that $t_+(y, \omega) \leq d$ for $(y, \omega, E) \in \Gamma_-$ since $\|\omega\| = 1$. Assume for simplicity that ∂G has parametrization (which is almost global), say $h : V \rightarrow \partial G \setminus \Gamma_1$ where Γ_1 has zero surface measure. Generally we have a finite number of parametrized patches that cover ∂G . Applying for each fixed ω the change of variables (in x -variable) $x = h(v) + t\omega =: H(v, t)$, we find that the Jacobian of J_H of H is

$$J_H(v, t) = \omega \cdot (\partial_1 h \times \partial_2 h) = \omega \cdot \nu(h(v)) \|(\partial_1 h \times \partial_2 h)(v)\|,$$

and that $H(W) = G$, where $W := \{(v, t) \mid v \in V_-, 0 < t < t_+(h(v), \omega)\}$ and $V_- := \{v \in V \mid \omega \cdot \nu(h(v)) < 0\}$. Hence we get

(90)

$$\begin{aligned}
\|Lg\|_{L^1(G \times S \times I)} &= \int_{G \times S \times I} |(Lg)(x, \omega, E)| dx d\omega dE \\
&= \int_{S \times I} \int_G |g(x - t(x, \omega)\omega, \omega, E)| dx d\omega dE \\
&= \int_{S \times I} \int_{V_-} \int_0^{t_+(h(v), \omega)} |g(h(v), \omega, E)| |J_H(v, t)| dt dv d\omega dE \\
&= \int_{S \times I} \int_{V_-} \int_0^{t_+(h(v), \omega)} |g(h(v), \omega, E)| |\omega \cdot \nu(h(v))| \|(\partial_1 h \times \partial_2 h)(v)\| dt dv d\omega dE \\
(91) \quad &\leq \int_{S \times I} \int_{V_-} \int_0^d |g(h(v), \omega, E)| |\omega \cdot \nu(h(v))| \|(\partial_1 h \times \partial_2 h)(v)\| dt dv d\omega dE \\
&= d \|g\|_{T^1(\Gamma_-)},
\end{aligned}$$

where in the third step we used that $t(h(v) + t\omega, \omega) = t$, while in the last step we noticed that $\|\partial_1 h \times \partial_2 h(v)\|$ is the Jacobian J_h of h , and that $h(V_-)$ differs from Γ_- only by a zero-measurable set (in fact $h(V_-) = \Gamma_- \setminus \{(y, \omega, E) \in \Gamma_1 \times S \times I\}$). This completes the proof. \square

As mentioned in section 2, the spaces $T^1(\Gamma_-)$ and $T^1(\Gamma_+)$ can be identified in a natural way. This is formulated in the following corollary.

Corollary 5.9 For every $g \in T^1(\Gamma_-)$ we have $(Lg)|_{\Gamma_+} \in T^1(\Gamma_+)$ and the map

$$\Theta_- : T^1(\Gamma_-) \rightarrow T^1(\Gamma_+); \quad g \mapsto (Lg)|_{\Gamma_+}$$

is an isometric isomorphism. In particular,

$$\|(Lg)|_{\Gamma_+}\|_{T^1(\Gamma_+)} = \|g\|_{T^1(\Gamma_-)}, \quad \forall g \in T^1(\Gamma_-).$$

Proof. It applies (9) with $u = L|g| = |Lg|$, recalls from Lemma 5.8 that $\omega \cdot \nabla_x(L|g|) = 0$, for $g \in T^1(\Gamma_-)$, and takes into account that the part Γ_0 of $\Gamma = \Gamma_0 \cup \Gamma_- \cup \Gamma_+$ is zero-measurable, one obtains

$$\begin{aligned}
0 &= \int_{G \times S \times I} \omega \cdot \nabla_x(L|g|) dx d\omega dE = \int_{\Gamma} L|g|(\omega \cdot \nu) d\sigma d\omega dE \\
&= - \int_{\Gamma_-} |g| |\omega \cdot \nu| d\sigma d\omega dE + \int_{\Gamma_+} |(Lg)|_{\Gamma_+} |\omega \cdot \nu| d\sigma d\omega dE \\
&= - \|g\|_{T^1(\Gamma_-)} + \|(Lg)|_{\Gamma_+}\|_{T^1(\Gamma_+)}.
\end{aligned}$$

This shows that the map Θ_- is isometric. By constructing the obvious inverse map of Θ_- shows that Θ_- is surjective as well. \square

Remark 5.10 Combining Lemma 5.8 and Corollary 5.9, we have the following bound for the lift operator L into the space $\tilde{W}^1(G \times S \times I)$:

$$\|Lg\|_{\tilde{W}^1(G \times S \times I)} \leq (d+2) \|g\|_{T^1(\Gamma_-)}.$$

As an immediate corollary of the Lemma 5.8, we have:

Lemma 5.11 Let $T > 0$ and $k \in \mathbb{N}_0$. Then for every $g \in C^k([0, T], T^1(\Gamma_-))$ there exists a lift $\psi = Lg \in C^k([0, T], \tilde{W}^1(G \times S \times I))$ such that $\gamma_-(Lg) = (Lg)|_{\Gamma_-} = g$. Moreover,

$$\nabla(Lg) = 0$$

and

$$\|Lg\|_{C^k([0, T], L^1(G \times S \times I))} = \|Lg\|_{C^k([0, T], W^1(G \times S \times I))} \leq d \|g\|_{C^k([0, T], T^1(\Gamma_-))}.$$

Proof. Defining the lift Lg by

$$(92) \quad (Lg)(x, \omega, E, t) = g(x - t(x, \omega)\omega, \omega, E, t),$$

we have $(Lg)(x, \omega, E, t) = L(g(t))(x, \omega, E)$, with the latter L the lift as defined in Lemma 5.8. As L of Lemma 5.8 is linear and bounded, it follows from $g \in C^k([0, T], T^1(\Gamma_-))$ that $Lg \in C^k([0, T], \tilde{W}^1(G \times S \times I))$, and for $j = 1, \dots, k$,

$$\|\partial_t^j(Lg)\|_{C([0, T], L^1(G \times S \times I))} = \|L(\partial_t^j g)\|_{C([0, T], L^1(G \times S \times I))} \leq d \|\partial_t^j g\|_{C([0, T], T^1(\Gamma_-))},$$

from which the desired estimate. \square

Example 5.12 If $G = B(0, r) \subset \mathbb{R}^3$ the lift L of Lemma 5.11 can be seen, due to Example 3.1, to be given by

$$(Lg)(x, \omega, E, t) = g\left(x - \left(\langle x, \omega \rangle + \sqrt{\langle x, \omega \rangle^2 + r^2 - \|x\|^2}\right)\omega, \omega, E, t\right),$$

for $g \in C^k([0, T], T^1(\Gamma_-))$.

Remark 5.13 Using Lemma 5.8 one can show that for any $1 \leq p < \infty$ and every $g \in T^p(\Gamma_-)$ has an extension $\psi = Lg \in \tilde{W}^p(G \times S \times I)$ such that $\gamma_-(Lg) = (Lg)|_{\Gamma_-} = g$. In addition, the linear lift operator $L : T^p(\Gamma_-) \rightarrow \tilde{W}^p(G \times S \times I)$ satisfies

$$(93) \quad \nabla(Lg) = 0$$

and

$$(94) \quad \|Lg\|_{L^p(G \times S \times I)} = \|Lg\|_{W^p(G \times S \times I)} \leq d \|g\|_{T^p(\Gamma_-)} \quad \text{for all } g \in T^p(\Gamma_-).$$

Indeed, the proof of (93) for any $1 \leq p < \infty$ proceeds precisely as in the case $p = 1$ (see the beginning of the proof of Lemma 5.8). On the other hand, if $g \in T^p(\Gamma_-)$ then $g^p \in T^1(\Gamma_-)$ and as $L(g^p) = (Lg)^p$, with Lg defined pointwise (a.e.) by (92), and hence (87) immediately implies (94). respectively.

Similarly, Lemma 5.11 admits a generalization to any $1 \leq p < \infty$.

For inhomogeneous inflow boundary data we get

Theorem 5.14 Suppose that the assumptions (67), (68) and (77) are valid. Then for every $f \in L^1(G \times S \times I)^3$ and $g \in T^1(\Gamma_-)^3$ the problem

$$(95) \quad \begin{aligned} \omega \cdot \nabla \psi_j + \Sigma_j \psi_j - K_j \psi &= f_j(x, \omega, E) \\ \psi_j|_{\Gamma_-} &= g_j, \end{aligned}$$

where $j = 1, 2, 3$, has a unique solution $\psi \in \tilde{W}^1(G \times S \times I)^3$.

Proof. As usual we apply the lift of inflow boundary data. By Lemma 5.8 there exists $\tilde{\psi}_j := Lg_j \in \tilde{W}^1(G \times S \times I)$ such that $\tilde{\psi}_j|_{\Gamma_-} = g_j$. Let $\tilde{\psi} = (\tilde{\psi}_1, \tilde{\psi}_2, \tilde{\psi}_3)$ and substitute in the problem (95) $u = \psi - \tilde{\psi}$ for ψ . Then we get

$$(96) \quad \begin{aligned} \omega \cdot \nabla u_j + \Sigma_j u_j - K_j u &= f_j - \omega \cdot \nabla \tilde{\psi}_j - \Sigma_j \tilde{\psi}_j + K_j \tilde{\psi} =: \tilde{f}_j(x, \omega, E) \\ u_j|_{\Gamma_-} &= \psi_j|_{\Gamma_-} - \tilde{\psi}_j|_{\Gamma_-} = g_j - g_j = 0, \end{aligned}$$

for $j = 1, 2, 3$. Since $\tilde{f} := (\tilde{f}_1, \tilde{f}_2, \tilde{f}_3) \in L^1(G \times S \times I)^3$ we get by Theorem 5.6 that the problem (96) has a unique solution $u \in \tilde{W}_{-,0}^1(G \times S \times I)^3$. Then $\psi := u + \tilde{\psi} \in \tilde{W}^1(G \times S \times I)^3$ is the required unique solution of (95) and so we obtain the assertion. \square

Corollary 5.15 Under the assumptions of Theorem 5.14 the solution ψ of the problem (95) satisfies, with some constants $C_1, C_2, C_3 > 0$, the estimates

$$(97) \quad \|\psi\|_{L^1(G \times S \times I)^3} \leq \frac{1}{c} \|f\|_{L^1(G \times S \times I)^3} + C_1 \|g\|_{T^1(\Gamma_-)^3},$$

$$(98) \quad \|\psi\|_{W^1(G \times S \times I)^3} \leq C_2 \left(\|f\|_{L^1(G \times S \times I)^3} + \|g\|_{T^1(\Gamma_-)^3} \right)$$

and

$$(99) \quad \|\psi\|_{\tilde{W}^1(G \times S \times I)^3} \leq C_3 \left(\|f\|_{L^1(G \times S \times I)^3} + \|g\|_{T^1(\Gamma_-)^3} \right)$$

Proof. By the proof of Theorem 5.14 $\psi = u + Lg$ where $u \in \tilde{W}_{-,0}^1(G \times S \times I)^3$ satisfies

$$(-\mathbf{A}_0 + \Sigma - K)u = f - (-\mathbf{A} + \Sigma - K)(Lg).$$

In addition, $\mathbf{A}(Lg) = 0$ by Lemma 5.8. Furthermore, by (86) and by Lemma 5.8

$$\begin{aligned} \|\psi\|_{L^1(G \times S \times I)^3} &= \|u + Lg\|_{L^1(G \times S \times I)^3} \\ &\leq \frac{1}{c} \|f - (\Sigma - K)(Lg)\|_{L^1(G \times S \times I)^3} + \|Lg\|_{L^1(G \times S \times I)^3} \\ &\leq \frac{1}{c} \left(\|f\|_{L^1(G \times S \times I)^3} + \|\Sigma - K\| d \|g\|_{T^1(\Gamma_-)^3} \right) + d \|g\|_{T^1(\Gamma_-)^3} \end{aligned}$$

which implies (97).

The assertion (98) follows from estimate (97) since $\omega \cdot \nabla \psi = f - (\Sigma - K)\psi$ when ψ is the solution of (95). Finally, the last estimate (99) follows from Theorem 2.6, which tells us that

$$\|\psi\|_{T^1(\Gamma_+)} \leq \|\psi\|_{W^1(G \times S \times I)^3} + \|\psi\|_{T^1(\Gamma_-)},$$

and from (98). This completes to proof. \square

The result of Corollary 5.15 means that the solution ψ depends continuously on the data f, g .

Finally we will consider the non-negativity of solutions. Since \mathbf{A}_0 is m -dissipative it generates a contraction C^0 -semigroup $T(t)$, $t \geq 0$ (Lumer-Phillips Theorem, see e.g. [18], p. 343, [21], pp. , [42], pp. 14-15, [25]). For $f \in D(\mathbf{A}_0) = \tilde{W}_{-,0}^1(G \times S \times I)^3$, the curve $\psi(t) = T(t)f$, $t > 0$, is the unique solution of the problem ([18], pp. 397-405, [42], p. 100, [25])

$$(100) \quad \frac{\partial \psi}{\partial t} - \mathbf{A}_0 \psi = 0, \quad \psi(0) = f$$

where $\psi \in C^1([0, \infty[, L^1(G \times S \times I)^3) \cap C([0, \infty[, \tilde{W}_{-,0}^1(G \times S \times I)^3)$.

Denote $\psi(x, \omega, E, t) := \psi(t)(x, \omega, E)$. The problem (100) can be solved (as above in Section 3.2) by the Lagrange's method in the classical sense which we describe shortly in the sequel assuming that f is sufficiently smooth, say $f \in C(\overline{G} \times S \times I) \cap D(\mathbf{A}_0)$. The equation (100) is uncoupled and for each j it is of the form

$$(101) \quad \frac{\partial \psi_j}{\partial t} + \sum_{k=1}^3 \omega_k \frac{\partial \psi_j}{\partial x_k} = 0$$

and ψ_j must satisfy an initial-boundary condition of the form

$$(102) \quad \begin{aligned} \psi_j(x, \omega, E, 0) &= f_j(x, \omega, E), & (x, \omega, E) &\in G \times S \times I, \\ \psi_j(y, \omega, E, t) &= 0, & (y, \omega, E, t) &\in \Gamma_- \times [0, \infty[. \end{aligned}$$

We solve the problem (101-102) for a fixed j and we denote for simplicity $\psi := \psi_j$ and $f := f_j$. Furthermore, denote $(x, \omega, E, t) = (x_1, x_2, x_3, \omega_1, \omega_2, \omega_3, E, t)$. Then the augmented system of ordinary differential equations (system of characteristics) is

$$(103) \quad \begin{aligned} T'(t) &= 1 \\ X'_1(s) &= \Omega_1, \quad \Omega'_1(s) = 0, \\ X'_2(s) &= \Omega_2, \quad \Omega'_2(s) = 0, \\ X'_3(s) &= \Omega_3, \quad \Omega'_3(s) = 0, \\ \mathcal{E}'(s) &= 0 \\ \Psi'(s) &= 0 \end{aligned}$$

We denote $X = (X_1, X_2, X_3)$, $\Omega = (\Omega_1, \Omega_2, \Omega_3)$. We find that

$$(104) \quad T(s) = s + C, \quad \Omega(s) = C', \quad X(s) = sC' + C'', \quad \mathcal{E}(s) = C''', \quad \Psi(s) = C''''$$

where C, C', C'', C''', C'''' are constants.

Taking into account the condition (102) we see that the solution of the augmented system must satisfy the initial condition of the form

$$(105) \quad \begin{aligned} (X(0), \Omega(0), \mathcal{E}(0), T(0), \Psi(0)) &= (h(v), \omega, E, t', 0), \quad t' > 0 \\ (X(0), \Omega(0), \mathcal{E}(0), T(0), \Psi(0)) &= (x', \omega, E, t', f(x', \omega, E)), \quad t' = 0 \end{aligned}$$

where $h = h(v)$ is as in Section 3.2 the local parametrization of ∂G . Here x (resp. t) is replaced by x' (resp. t') for notational reasons. Matching the initial condition (105) to the solution (104) we get the solution $(X(s), \Omega(s), \mathcal{E}(s), T(s), \Psi(s))$. By eliminating x', v, t', E, ω from the system

$$\begin{aligned} (X(s), \Omega(s), \mathcal{E}(s), T(s), \Psi(s)) &= (x, \omega, E, t, 0) \text{ for } t' > 0 \\ (X(s), \Omega(s), \mathcal{E}(s), T(s), \Psi(s)) &= (x, \omega, E, t, f(x, \omega, E)) \text{ for } t' = 0 \end{aligned}$$

and noting that (formally)

$$\Psi(s) = H(-t')f(x', \omega, E)$$

we get the solution ψ as in Section 3.2. The result is

$$(106) \quad \psi(x, \omega, E, t) = f(x - t\omega, \omega, E)H(t(x, \omega) - t), \quad f \in \tilde{W}_{-,0}^1(G \times S \times I) \cap C(\overline{G} \times S \times I)$$

where H is the Heaviside function. Applying the limiting techniques (cf. the proof of Theorem 4.7) we get

(107)

$$(T(t)f)(x, \omega, E) = \psi(t)(x, \omega, E) = H(t(x, \omega) - t)f(x - t\omega, \omega, E), \quad f \in \tilde{W}_{-,0}^1(G \times S \times I).$$

Since $\tilde{W}_{-,0}^1(G \times S \times I)$ is dense in $L^1(G \times S \times I)$ the formula (107) is valid for any $f \in L^1(G \times S \times I)$.

For the three particles the semigroup $T(t)$ is given by

$$(108) \quad \begin{aligned} & (T(t)f)(x, \omega, E) \\ &= H(t(x, \omega) - t)(f_1(x - t\omega, \omega, E), f_2(x - t\omega, \omega, E), f_3(x - t\omega, \omega, E)), \end{aligned}$$

where $f \in L^1(G \times S \times I)^3$. In literature (see e.g. [19], pp. 222-224), the formula (108) is demonstrated for one particle system by using different methods.

We have the following result on non-negativity of solutions.

Theorem 5.16 Suppose that the assumptions of Theorem 5.14 are valid and that moreover

$$(109) \quad \begin{aligned} & f_j(x, \omega, E) \geq 0 \text{ a.e. } (x, \omega, E) \in G \times S \times I \\ & g_j(y, \omega, E) \geq 0 \text{ a.e. } (y, \omega, E) \in \Gamma_-, \text{ for } j = 1, 2, 3. \end{aligned}$$

Then the solution given in Theorem 5.14 satisfies $\psi(x, \omega, E) \geq 0$ a.e. $(x, \omega, E) \in G \times S \times I$.

Proof. A. We put the problem (95) in the abstract form

$$(110) \quad \begin{aligned} & -\mathbf{A}\psi + \Sigma\psi - K\psi = f, \\ & \psi|_{\Gamma_-} = g. \end{aligned}$$

Assume at first that $g = 0$. Then the problem (110) is $(-\mathbf{A}_0 + \Sigma - K)\psi = f$. Let, as above, $T(t)$ be the C^0 -semigroup generated by \mathbf{A}_0 . Then by (108)

$$T(t)f \geq 0 \text{ for } f \geq 0$$

In addition, we immediately see that

$$K\psi \geq 0 \text{ for } \psi \geq 0,$$

and that

$$(\Sigma_j\psi)(x, \omega, E) = \Sigma_j(x, \omega, E)\psi_j(x, \omega, E) \geq 0 \text{ for } \psi \geq 0,$$

a.e. $(x, \omega, E) \in G \times S \times I$, as $\Sigma_j(x, \omega, E) \geq 0$ by assumption. These imply that if T_K and $T_{-\Sigma}$ are the semigroups generated by the bounded operators K and $-\Sigma$, i.e. $T_K(t)\psi = \sum_{i=0}^{\infty} \frac{1}{i!} t^i K^i \psi$ and $T_{-\Sigma}(t)\psi = (e^{-t\Sigma_1}\psi_1, e^{-t\Sigma_2}\psi_2, e^{-t\Sigma_3}\psi_3)$, we have $T_K\psi \geq 0$, $T_{-\Sigma}\psi \geq 0$ whenever $\psi \geq 0$.

Since by the proof of Theorem 5.6 $\mathbf{A}_0 - (\Sigma - K) + cI$ is m -dissipative, the operator $\mathbf{A}_0 - \Sigma + K$ generates a contraction C^0 -semigroup $G(t)$ for which in addition

$$\|G(t)\| \leq e^{-c't}, \quad \forall t \geq 0,$$

where c' is a positive number which is less than or equal to $c > 0$. Note here that the m -dissipative operator $\mathbf{A}_0 - (\Sigma - K) + c'I$ generates the semigroup $e^{c't}G(t)$. This is a consequence of the Lumer-Phillips Theorem ([18], p. 343, [21], Theorem II.3.15, p. 83 and [25]). From Hille-Yosida Theorem ([18], p. 321 and [21], Theorem II.3.5,

p. 73) and from the resolvent formula (cf. [21], Theorem II.1.10, p. 55) we obtain that

$$(111) \quad \begin{aligned} \psi &= (-\mathbf{A}_0 + \Sigma - K)^{-1} f = (c'I - (\mathbf{A}_0 - (\Sigma - K) + c'I))^{-1} \\ &= \int_0^\infty e^{-c't} (e^{c't} G(t)) f dt = \int_0^\infty G(t) f dt. \end{aligned}$$

By the Trotter's formula ([21], Theorem III.5.2, p. 220, or [25], p.53, where the proof is given only for contraction semigroups)

$$G(t)f = \lim_{n \rightarrow \infty} (T(t/n)T_{-\Sigma}(t/n)T_K(t/n))^n f$$

which implies that $G(t)f \geq 0$ for $f \geq 0$ (cf. Section XXI-§2, Proposition 2, pp. 226-227 of [19]). Hence $\psi \geq 0$ and then the proof is complete in this special case.

B. Suppose that more generally $g \in T^1(\Gamma_-)^3$ is such that $g \geq 0$. By Theorem 5.14 the solution $u \in \tilde{W}^1(G \times S \times I)^3$ of the problem

$$(112) \quad -\mathbf{A}u + \Sigma u = 0, \quad u|_{\Gamma_-} = g,$$

exists. We show that it is non-negative. Indeed, applying again limiting techniques we find that by (49) the (distributional) solution is

$$(113) \quad \begin{aligned} u(x, \omega, E) &= \left(e^{\int_0^{t(x, \omega)} \Sigma_1(x-s\omega, \omega, E) ds} \cdot g_1(x - t(x, \omega)\omega, \omega, E), \right. \\ &\quad e^{\int_0^{t(x, \omega)} \Sigma_2(x-s\omega, \omega, E) ds} \cdot g_2(x - t(x, \omega)\omega, \omega, E), \\ &\quad \left. e^{\int_0^{t(x, \omega)} \Sigma_3(x-s\omega, \omega, E) ds} \cdot g_3(x - t(x, \omega)\omega, \omega, E) \right), \end{aligned}$$

from which one immediately sees that $u \geq 0$ once $g \geq 0$.

Finally, let $w := \psi - u$. Then we find that

$$(114) \quad \begin{aligned} -\mathbf{A}w + \Sigma w - Kw &= f + (\mathbf{A}u - \Sigma u + Ku) = f + Ku \geq 0 \\ w|_{\Gamma_-} &= g - g = 0. \end{aligned}$$

Hence by Part A. of the proof, we have $w \geq 0$ and therefore $\psi = w + u \geq 0$. This completes the proof. \square

Remark 5.17 Consider the transport problem (95). The solution $\psi \in \tilde{W}^1(G \times S \times I)^3$ can be decomposed as follows. Let $u \in \tilde{W}^1(G \times S \times I)^3$ be the solution of the problem

$$(115) \quad \omega \cdot \nabla u_j + \Sigma_j u_j = f_j, \quad \text{on } G \times S \times I, \quad j = 1, 2, 3,$$

together with the inflow boundary condition

$$(116) \quad u|_{\Gamma_-} = g.$$

Furthermore, let $w \in \tilde{W}^1(G \times S \times I)^3$ be the solution of the problem

$$(117) \quad \omega \cdot \nabla w_j + \Sigma_j w_j - K_j w = K_j u, \quad \text{on } G \times S \times I, \quad j = 1, 2, 3,$$

with the homogeneous inflow boundary values

$$(118) \quad w|_{\Gamma_-} = 0.$$

Then we find that $\psi = u + w \in \tilde{W}^1(G \times S \times I)^3$ is the solution of (95). This decomposition is corresponding to the evolution of primary particles (u) and of secondary particles (w) of the overall particle transport. The decomposition $\psi = u + w$ may be useful e.g. in constructing numerical solutions. Note that *the system*

(115)-(116) is uncoupled. By (46) we formally have an explicit solution for (115)-(116)

$$(119) \quad \begin{aligned} u_j(x, \omega, E) = & \int_0^{t(x, \omega)} e^{\int_0^t -\Sigma_j(x-s\omega, \omega, E) ds} f_j(x-t\omega, \omega, E) dt \\ & + e^{\int_0^{t(x, \omega)} -\Sigma_j(x-s\omega, \omega, E) ds} g_j(x-t(x, \omega)\omega, \omega, E). \end{aligned}$$

Remark 5.18 By the proof of Theorem 5.14 the solution ψ of the transport problem

$$(-\mathbf{A} + \Sigma - K)\psi = f, \quad \psi|_{\Gamma_-} = g$$

is the sum (recall that $\mathbf{A}(Lg) = 0$)

$$(120) \quad \begin{aligned} \psi = u + Lg = & (-\mathbf{A}_0 + \Sigma - K)^{-1}(f - (-\mathbf{A} + \Sigma - K)(Lg)) + Lg \\ = & (-\mathbf{A}_0 + \Sigma - K)^{-1}(f - (\Sigma - K)(Lg)) + Lg. \end{aligned}$$

Since Lg is known, the essential part from the computational point of view is to find u that is the solution of the equation

$$(-\mathbf{A}_0 + \Sigma - K)u = f - (\Sigma - K)(Lg) =: \tilde{f}.$$

We see, on the other hand, that this equation is equivalent to

$$(-\mathbf{A}_0 + \Sigma)u = Ku + \tilde{f}$$

or to (notice that $(-\mathbf{A}_0 + \Sigma)^{-1}$ exists)

$$u = (-\mathbf{A}_0 + \Sigma)^{-1}Ku + (-\mathbf{A}_0 + \Sigma)^{-1}\tilde{f}.$$

This can, furthermore, be written into the form

$$(121) \quad (I - T)u = \tilde{\tilde{f}}$$

where $T := (-\mathbf{A}_0 + \Sigma)^{-1}K$ is a bounded linear operator from $L^1(G \times S \times I)^3$ into itself, and $\tilde{\tilde{f}} := (-\mathbf{A}_0 + \Sigma)^{-1}\tilde{f}$.

If it happened that $\|T\| < 1$, the solution u would be obtained from the Neumann series

$$(122) \quad u = \sum_{k=0}^{\infty} T^k \tilde{\tilde{f}} = \sum_{k=0}^{\infty} ((-\mathbf{A}_0 + \Sigma)^{-1}K)^k ((-\mathbf{A}_0 + \Sigma)^{-1}(f - (\Sigma - K)(Lg))),$$

where by (50) the j -th component, $j = 1, 2, 3$, of $(-\mathbf{A}_0 + \Sigma)^{-1}h$ is for any $h \in L^1(G \times S \times I)$ given by (in generalized sense; see (66))

$$(123) \quad ((-\mathbf{A}_0 + \Sigma)^{-1}h)_j = \int_0^{t(x, \omega)} e^{\int_0^t -\Sigma_j(x-s\omega, \omega, E) ds} h_j(x-t\omega, \omega, E) dt.$$

From the computational point of view, this approach, or rather a discretized version of it, has the advantage that no explicit inversions of matrices are needed. The condition $\|T\| < 1$ is, however, restrictive. For $p = \infty$ a sufficient condition for having $\|T\| < 1$ is that for $j = 1, 2, 3$ (we omit all details here)

$$\Sigma_j(x, \omega, E) \geq c > 0$$

and for some $0 < \beta < 1$ and a.e. on $G \times S \times I$,

$$\beta \Sigma_j(x, \omega, E) \geq \sum_{k=1}^3 \int_S \int_I \sigma_{jk}(x, \omega, \omega', E, E') d\omega' dE',$$

which is stronger a condition to satisfy than (77). In addition, the data (f, g) must be in the corresponding L^∞ -spaces (cf. [19], pp. 243-244, in the case of one species of particles). We refer also to [15], Prop. 2.3, where a sufficient condition to have $\|T\| < 1$ is given in the case where $p = 1$ and one species of particles is considered.

Remark 5.19 Another method to compute approximately the solution of the problem

$$(124) \quad (-\mathbf{A}_0 + \Sigma - K)u = f - (\Sigma - K)(Lg) =: \tilde{f},$$

which avoids the explicit inversions of matrices, can be described as follows. By the Trotter's formula, the semigroup $G(t)$ generated by $\mathbf{A}_0 - \Sigma + K$ is given by (see the proof of Theorem 5.16 above)

$$(125) \quad G(t)f = \lim_{n \rightarrow \infty} (T(t/n)T_{-\Sigma}(t/n)T_K(t/n))^n f, \quad (t \geq 0)$$

and the limit is uniform on compact intervals $[0, T]$. We know that

$$(126) \quad \begin{aligned} T(t)f &= H(t(x, \omega) - t)(f_1(x - t\omega, \omega, E), f_2(x - t\omega, \omega, E), f_3(x - t\omega, \omega, E)) \\ T_{-\Sigma}(t)f &= e^{-t\Sigma(x, \omega, E)} f = (e^{-t\Sigma_1(x, \omega, E)} f_1, e^{-t\Sigma_2(x, \omega, E)} f_2, e^{-t\Sigma_3(x, \omega, E)} f_3) \\ T_K(t)f &= e^{tK} f = \sum_{k=0}^{\infty} \frac{1}{k!} (tK)^k f \approx \sum_{k=0}^{N_0} \frac{1}{k!} (tK)^k f. \end{aligned}$$

In virtue of formula (111)

$$(127) \quad \begin{aligned} \psi &= \int_0^\infty G(t)\tilde{f}dt \approx \int_0^T G(t)\tilde{f}dt = \int_0^T \lim_{n \rightarrow \infty} (T(t/n)T_{-\Sigma}(t/n)T_K(t/n))^n \tilde{f}dt \\ &\approx \int_0^T [T(t/n_0)T_{-\Sigma}(t/n_0)T_K(t/n_0)]^{n_0} \tilde{f}dt \\ &= \int_0^T \left[T(t/n_0) e^{-(t/n_0)\Sigma(x, \omega, E)} \sum_{k=0}^{N_0} \frac{1}{k!} ((t/n_0)K)^k \right]^{n_0} \tilde{f}dt \end{aligned}$$

where T , n_0 and N_0 are large enough. Note that the result in (127) can be immediately computed since $T(t)$ is explicitly known.

This approach, unlike the one given in Remark 5.18, does not require extra assumptions on cross-sections.

6. ON TIME-DEPENDENT SOLUTIONS FOR THE COUPLED SYSTEM

In this section we do not need the assumption (77) since for time-dependent equations only the C^0 -semigroup property is essential. The contraction property of semigroup is not needed.

We have $E = \frac{1}{2}m_j \|v_j\|^2$ where m_j (resp. $\|v_j\|$) is the mass (resp. the speed) of the particle j . Hence $\|v_j\| = \sqrt{\frac{2E}{m_j}}$. In the following we consider the problem (for $\|v_j\| \neq 0$),

$$\begin{aligned} \frac{1}{\|v_j\|} \frac{\partial \psi_j}{\partial t} + \omega \cdot \nabla \psi_j + \Sigma_j \psi - K_j \psi &= f_j(x, \omega, E, t), & (x, \omega, E) \in G \times S \times I, \quad t \in]0, T] \\ \psi(y, t) &= g_j(y, t), & y \in \Gamma_-, \quad t \in]0, T] \\ \psi_j(x, \omega, E, 0) &= \psi_0(x, \omega, E), & (x, \omega, E) \in G \times S \times I \end{aligned}$$

where $j = 1, 2, 3$, $T > 0$ and $\psi_j = \psi_j(t)(x, \omega, E) = \psi_j(x, \omega, E, t)$ (we use this agreement without further mention). Multiplying the above transport equation by $\|v_j\|$ we obtain the equation

$$(128) \quad \frac{\partial \psi_j}{\partial t} + v_j \cdot \nabla \psi_j + \tilde{\Sigma}_j \psi - \tilde{K}_j \psi = \tilde{f}_j, \quad (x, \omega, E, t) \in G \times S \times I \times]0, T[$$

$$(129) \quad \psi(y, t) = g(y, t), \quad y \in \Gamma_-, \quad t \in]0, T[$$

$$(130) \quad \psi(x, \omega, E, 0) = \psi_0(x, \omega, E), \quad (x, \omega, E) \in G \times S \times I$$

where v_j is the velocity $\|v_j\| \omega = \sqrt{\frac{2E}{m_j}} \omega$ of the j -th particle, and where $\tilde{\Sigma}_j = \sqrt{\frac{2E}{m_j}} \Sigma_j$, \tilde{K} is the collision operator corresponding to the cross-sections $\tilde{\sigma}_{kj} = \sqrt{\frac{2E}{m_j}} \sigma_{kj}$ and $\tilde{f}_j = \sqrt{\frac{2E}{m_j}} f_j$.

We modify slightly the function spaces given in section 2. Let

$$\mathcal{W}^1(G \times S \times I) = \{\psi \in L^1(G \times S \times I) \mid \sqrt{E} \omega \cdot \nabla \psi \in L^1(G \times S \times I)\}.$$

Then by standard arguments $\mathcal{W}^1(G \times S \times I)$ equipped with the norm

$$\|\psi\|_{\mathcal{W}^1(G \times S \times I)} = \|\psi\|_{L^1(G \times S \times I)} + \left\| \sqrt{E} \omega \cdot \nabla \psi \right\|_{L^1(G \times S \times I)}.$$

is a Banach space and $\mathcal{D}(\overline{G} \times S \times I)$ is dense subspace of it.

Furthermore we define

$$\mathcal{T}^1(\Gamma_-) = L^1(\Gamma_-, \sqrt{E} |\omega \cdot \nu| \, d\sigma d\omega dE)$$

with the norm

$$\|h\|_{\mathcal{T}^1(\Gamma_-)} = \int_{\Gamma_-} |h(y, \omega, E)| \sqrt{E} |\omega \cdot \nu| \, d\sigma d\omega dE.$$

The space $\mathcal{T}^1(\Gamma_+)$ is defined similarly. Again any element $\psi \in \mathcal{W}^1(G \times S \times I)$ has well defined trace $\psi|_{\Gamma_-}$ in $L^1_{\text{loc}}(\Gamma_-, \sqrt{E} |\omega \cdot \nu| \, d\sigma d\omega dE)$ and the trace mapping $\gamma_- : \mathcal{W}^1(G \times S \times I) \rightarrow L^1_{\text{loc}}(\Gamma_-, \sqrt{E} |\omega \cdot \nu| \, d\sigma d\omega dE)$; $\gamma_-(\psi) = \psi|_{\Gamma_-}$ is continuous. Similarly for the trace γ_+ on the outflow boundary Γ_+ , and we can define the trace $\gamma(\psi) = \psi|_{\Gamma}$ on the whole Γ as in section 2.

We denote by $\mathcal{T}^1(\Gamma)$ the space of L^1 -functions with respect to the measure $\sqrt{E} |\omega \cdot \nu| \, d\sigma d\omega dE$, and equip it with the norm

$$\|h\|_{\mathcal{T}^1(\Gamma)} = \int_{\Gamma} |h(y, \omega, E)| \sqrt{E} |\omega \cdot \nu| \, d\sigma d\omega dE.$$

Finally we define

$$\tilde{\mathcal{W}}^1(G \times S \times I) = \{\psi \in \mathcal{W}^1(G \times S \times I) \mid \gamma(\psi) \in \mathcal{T}^1(\Gamma)\},$$

which is again a Banach space with respect to the norm

$$\|\psi\|_{\tilde{\mathcal{W}}^1(G \times S \times I)} = \|\psi\|_{\mathcal{W}^1(G \times S \times I)} + \|\gamma(\psi)\|_{\mathcal{T}^1(\Gamma)},$$

and denote its subspace of elements of zero trace on the inflow boundary Γ_- by

$$\tilde{\mathcal{W}}^1_{-,0}(G \times S \times I) = \{\psi \in \mathcal{W}^1(G \times S \times I) \mid \gamma_-(\psi) = 0\}.$$

Define closed operators $\tilde{\mathbf{A}}, \tilde{\mathbf{A}}_0 : L^1(G \times S \times I)^3 \rightarrow L^1(G \times S \times I)^3$ by

$$\begin{aligned} \tilde{\mathbf{A}}\psi &:= (-v_1 \cdot \nabla \psi_1, -v_2 \cdot \nabla \psi_2, -v_3 \cdot \nabla \psi_3), \\ &= \left(-\sqrt{\frac{2E}{m_1}} \omega \cdot \nabla \psi_1, -\sqrt{\frac{2E}{m_2}} \omega \cdot \nabla \psi_2, -\sqrt{\frac{2E}{m_3}} \omega \cdot \nabla \psi_3 \right), \quad \psi \in D(\tilde{\mathbf{A}}) := \mathcal{W}^1(G \times S \times I)^3 \end{aligned}$$

and

$$\tilde{\mathbf{A}}_0\psi := \tilde{\mathbf{A}}\psi, \quad \psi \in D(\tilde{\mathbf{A}}_0) := \tilde{\mathcal{W}}_{-,0}^1(G \times S \times I)^3.$$

In addition, let $\tilde{\Sigma}\psi = (\tilde{\Sigma}_1\psi, \tilde{\Sigma}_2\psi, \tilde{\Sigma}_3\psi)$ and $\tilde{K}\psi = (\tilde{K}_1\psi, \tilde{K}_2\psi, \tilde{K}_3\psi)$.

Assuming that (67) and (68) hold we see similarly as in section 5.1 that the operators $\tilde{\Sigma}$ and \tilde{K} are bounded operators $L^1(G \times S \times I)^3 \rightarrow L^1(G \times S \times I)^3$. In addition, the operator $\tilde{\mathbf{A}}_0 : L^1(G \times S \times I)^3 \rightarrow L^1(G \times S \times I)^3$ is m -dissipative. In fact, the equation $(\lambda I - \tilde{\mathbf{A}}_0)\psi = \tilde{f}$ is nothing more than

$$\sqrt{\frac{2E}{m_j}}\omega \cdot \nabla \psi_j + \lambda \psi_j = \tilde{f}_j, \quad \psi_j|_{\Gamma_-} = 0, \quad j = 1, 2, 3,$$

or equivalently for $E > 0$

$$\begin{aligned} \omega \cdot \nabla \psi_j + \lambda \sqrt{\frac{m_j}{2E}}\psi_j &= \sqrt{\frac{m_j}{2E}}\tilde{f}_j \\ \psi_j|_{\Gamma_-} &= 0, \quad j = 1, 2, 3 \end{aligned}$$

whose solution for each j is, by sections 3.3 and 4 (see (38), (66)),

$$\psi_j = \sqrt{\frac{m_j}{2E}} \int_0^{t(x,\omega)} e^{-\lambda t \sqrt{m_j/(2E)}} \tilde{f}_j(x - \omega t, \omega, E) dt.$$

Similarly as in sections 4.2 and 5.1 we see that

$$\left\| (\lambda I - \tilde{\mathbf{A}}_0)\psi \right\|_{L^1(G \times S \times I)^3} \geq \lambda \|\psi\|_{L^1(G \times S \times I)^3}, \quad \psi \in D(\tilde{\mathbf{A}}_0)$$

and that $R(\lambda I - \tilde{\mathbf{A}}_0) = L^1(G \times S \times I)^3$. Hence $\tilde{\mathbf{A}}_0$ is m -dissipative.

Since $\tilde{\mathbf{A}}_0$ is m -dissipative and $\tilde{\Sigma} - \tilde{K}$ is bounded, the operator $\tilde{\mathbf{A}}_0 - \tilde{\Sigma} + \tilde{K} : L^1(G \times S \times I)^3 \rightarrow L^1(G \times S \times I)^3$ generates a C^0 -semigroup, which we denote by $\tilde{G}(t)$ ([18], p. 348, [21], Theorem III.1.3., pp. 158, [25] and [42], pp. 76-77) and which satisfies the estimate

$$\left\| \tilde{G}(t) \right\| \leq e^{\|\tilde{\Sigma} - \tilde{K}\|t}, \quad \forall t \geq 0.$$

We get the following standard result from the theory of abstract Cauchy problems for $g = 0$.

Theorem 6.1 Suppose that the assumptions (67) and (68) are valid. Furthermore, suppose that $\tilde{f} \in C^1([0, T], L^1(G \times S \times I)^3)$ and $\psi_0 \in D(\tilde{\mathbf{A}}_0) = \tilde{\mathcal{W}}_{-,0}^1(G \times S \times I)^3$. Then the problem (128)-(130) for $g = 0$ has a unique solution

$$(131) \quad \psi \in C^1([0, T], L^1(G \times S \times I)^3) \cap C([0, T], \mathcal{W}^1(G \times S \times I)^3),$$

such that

$$(132) \quad \psi(t) \in D(\tilde{\mathbf{A}}_0) = \tilde{\mathcal{W}}_{-,0}^1(G \times S \times I)^3 \text{ for all } t \geq 0.$$

Moreover, this solution is given by

$$(133) \quad \psi(t) = \tilde{G}(t)\psi_0 + \int_0^t \tilde{G}(t-s)\tilde{f}(s)ds.$$

Proof. Theorem follows from the solution theory of abstract Cauchy problems. See e.g. [18], pp. 397-400, [21], Corollary VI.7.6., pp. 439, [25], [42], pp. 105-108. \square

The next theorem includes a non-zero inflow boundary data.

Theorem 6.2 Suppose that the assumptions (67) and (68) are valid. Furthermore, suppose that $\tilde{f} \in C^1([0, T], L^1(G \times S \times I)^3)$, $\psi_0 \in \tilde{\mathcal{W}}^1(G \times S \times I)^3$ and $g \in C^2([0, T], \mathcal{T}^1(\Gamma_-)^3)$ such that

$$(134) \quad g(0) = \psi_0|_{\Gamma_-}.$$

Then the problem (128)-(130) has a unique solution

$$(135) \quad \psi \in C^1([0, T], L^1(G \times S \times I)^3) \cap C([0, T], \mathcal{W}^1(G \times S \times I)^3)$$

such that

$$(136) \quad \psi(t)|_{\Gamma_-} = g(t), \text{ for all } t \geq 0.$$

The condition (134) is called a *compatibility condition*: one must have $g(y, \omega, E, 0) = \psi_0(y, \omega, E)$ for a.e. $(y, \omega, E) \in \Gamma_-$.

Proof. Similarly as in Lemma 5.11 for each j there exists a lift

$$\tilde{\psi}_j = Lg_j \in C^2([0, T], \tilde{\mathcal{W}}^1(G \times S \times I))$$

such that $\tilde{\psi}_j|_{\Gamma_- \times [0, T]} = g_j$.

Define $\tilde{\psi} = (\tilde{\psi}_1, \tilde{\psi}_2, \tilde{\psi}_3)$ and substitute $u = \psi - \tilde{\psi}$ for ψ in problem (128)-(130) to obtain

$$(137) \quad \begin{aligned} \frac{\partial u_j}{\partial t} + v_j \cdot \nabla u_j + \tilde{\Sigma}_j u - \tilde{K}_j u \\ = \tilde{f}_j - \frac{\partial \tilde{\psi}_j}{\partial t} - v_j \cdot \nabla \tilde{\psi}_j - \tilde{\Sigma}_j \tilde{\psi} + \tilde{K}_j \tilde{\psi} =: \bar{f}_j \quad \text{on } G \times S \times I \times]0, T] \\ u(y, t) = g(y, t) - g(y, t) = 0 \quad \text{on } \Gamma_- \times]0, T] \\ u(\cdot, 0) = \psi_0 - \tilde{\psi}(0) \in \tilde{\mathcal{W}}_{-,0}^1(G \times S \times I)^3 \quad \text{on } G \times S \times I. \end{aligned}$$

Notice that in the last step we have by the compatibility condition $\tilde{\psi}(0)|_{\Gamma_-} = (Lg)(0)|_{\Gamma_-} = g(0) = \psi_0|_{\Gamma_-}$ and therefore $u(\cdot, 0) \in \tilde{\mathcal{W}}_{-,0}^1(G \times S \times I)^3$ (here $Lg = (Lg_1, Lg_2, Lg_3)$). In addition we find that $\bar{f}_j \in C^1([0, T], L^1(G \times S \times I)^3)$ (we omit the details here). By Theorem 6.1 the problem (137) has a unique solution

$$u \in C([0, T], L^1(G \times S \times I)^3) \cap C^1([0, T], L^1(G \times S \times I)^3) \cap C([0, T], \mathcal{W}^1(G \times S \times I)^3)$$

such that $u(t) \in \tilde{\mathcal{W}}_{-,0}^1(G \times S \times I)^3$ for $t \geq 0$. Then $\psi := u + \tilde{\psi}$ is the required unique solution of the problem (128)-(130) and the proof is complete. \square

The non-negativity of solutions in this dynamical case follows as above for steady state solutions. Here we denote $f_j(x, \omega, E, t) = f_j(t)(x, \omega, E)$ and so on. We have

Theorem 6.3 Suppose that the assumptions of Theorem 6.2 are valid and that moreover for $j = 1, 2, 3$,

$$(138) \quad f_j(x, \omega, E, t) \geq 0, \quad \text{for } t \geq 0 \text{ and a.e. } (x, \omega, E) \in G \times S \times I$$

$$(139) \quad g_j(y, \omega, E, t) \geq 0, \quad \text{for } t \geq 0 \text{ and a.e. } (y, \omega, E) \in \Gamma_-,$$

$$(140) \quad \psi_0(x, E, \omega) \geq 0, \quad \text{for a.e. } (x, \omega, E) \in G \times S \times I.$$

Then the solution of the problem (128)-(130) given in Theorem 6.2 satisfies $\psi(x, \omega, E, t) \geq 0$ for $t \geq 0$ and a.e. $(x, \omega, E) \in G \times S \times I$.

Proof. The problem (128)-(130) has the form

$$(141) \quad \frac{\partial \psi}{\partial t} - \tilde{\mathbf{A}}\psi + \tilde{\Sigma}\psi - \tilde{K}\psi = \tilde{f},$$

$$(142) \quad \psi|_{\Gamma_- \times]0, T]} = g$$

$$(143) \quad \psi(0) = \psi_0.$$

A. In the first step, we assume that $g = 0$ (then by the assumptions of Theorem 6.2 $\psi_0 \in D(\tilde{\mathbf{A}}_0)$). Let $\tilde{T}(t)$ be the C^0 -semigroup generated by $\tilde{\mathbf{A}}_0$. Then one has

$$\tilde{T}(t)f \geq 0 \quad \text{for all } f \in L^1(G \times S \times I)^3 \text{ such that } f \geq 0.$$

Indeed, according to what was done in section 5.3, one has

$$(T(t)f)(x, \omega, E) = ((T_1(t)f_1)(x, \omega, E), (T_2(t)f_2)(x, \omega, E), (T_3(t)f_3)(x, \omega, E))$$

where (see (108))

$$(T_j(t)f_j)(x, \omega, E) = H\left(t(x, \omega) - t\sqrt{\frac{2E}{m_j}}\right) \tilde{f}_j\left(x - \omega\sqrt{\frac{2E}{m_j}}t, \omega, E\right), \quad j = 1, 2, 3$$

for $\tilde{f} \in L^1(G \times S \times I)^3$.

Moreover, we have

$$\tilde{K}\psi \geq 0 \text{ for } \psi \in L^1(G \times S \times I)^3; \psi \geq 0$$

and $\tilde{\Sigma} \in L^\infty(G \times S \times I)^3$ such that $\tilde{\Sigma}_j \geq 0$. Since $\tilde{K} : L^1(G \times S \times I)^3 \rightarrow L^1(G \times S \times I)^3$ is a bounded operator we obtain, as earlier in the proof of Theorem 5.16, by Trotter's formula that $\tilde{G}(t)\tilde{f} \geq 0$ for $\tilde{f} \geq 0$ (cf. also Proposition 2 of [19], pp. 226-227), which implies that

$$(144) \quad \psi = \tilde{G}(t)\psi_0 + \int_0^t \tilde{G}(t-s)\tilde{f}(s)ds \geq 0.$$

Hence the assertion of the theorem is true for $g = 0$.

B. Suppose more generally that $g \in C^2([0, T], \mathcal{T}^1(\Gamma_-)^3)$ and $g \geq 0$. We see (cf. [19], pp. 231-232) that the solution $u \in C^0([0, T], L^1(G \times S \times I)^3) \cap C^1([0, T], L^1(G \times S \times I)^3)$ of the problem (which exists at least if $g(0) = 0$)

$$(145) \quad \frac{\partial u}{\partial t} - \tilde{\mathbf{A}}u + \tilde{\Sigma}u = 0, \quad u|_{\Gamma_- \times]0, T]} = g, \quad u(0) = 0$$

is non-negative. Again the problem (145) can be solved (as above in Section 3.2) by the Lagrange's method in the classical sense which we describe briefly in what follows, assuming that g is sufficiently smooth, say $g \in C(\overline{G} \times S \times I \times [0, T])^3$, and that g_j is zero in a neighbourhood of the surfaces given by the equation $t = t(x, \omega)\sqrt{\frac{m_j}{2E}}$ for $E > 0$ in the phase space $\overline{G} \times S \times I \times [0, T]$. For a general g then, the *mild* (generalized) solution is obtained by standard limiting processes (cf. the end of section 4.2).

The equation (145) is uncoupled and for each j it is of the form (we assume $E > 0$)

$$(146) \quad \sqrt{\frac{m_j}{2E}} \frac{\partial u_j}{\partial t} + \sum_{k=1}^3 \omega_k \frac{\partial u_j}{\partial x_k} + \Sigma_j(x, \omega, E)u_j = 0$$

and u_j must satisfy an initial-boundary condition of the form

$$(147) \quad \begin{aligned} u_j(x, \omega, E, 0) &= 0 & \text{for } (x, \omega, E) \in G \times S \times I, \\ u_j(y, \omega, E, t) &= g_j(y, \omega, E, t) & \text{for } (y, \omega, E, t) \in \Gamma_- \times]0, T]. \end{aligned}$$

We solve the problem (146)-(147) for a fixed j and we denote for simplicity $u := u_j$ and $m := m_j$, $g := g_j$. The augmented system of ordinary differential equations is

$$\begin{aligned}
 T'(t) &= \sqrt{\frac{m}{2E}} \\
 X'_1(s) &= \Omega_1, \quad \Omega'_1(s) = 0, \\
 X'_2(s) &= \Omega_2, \quad \Omega'_2(s) = 0, \\
 X'_3(s) &= \Omega_3, \quad \Omega'_3(s) = 0, \\
 \mathcal{E}'(s) &= 0 \\
 U'(s) &= -\Sigma(X, \Omega, E)U
 \end{aligned}
 \tag{148}$$

We find that

$$\begin{aligned}
 T(s) &= \sqrt{\frac{m}{2E}}s + C_1, \quad \Omega(s) = C_2, \quad X(s) = C_2s + C_3, \quad \mathcal{E}(s) = C_4, \\
 \Psi(s) &= C_5 e^{\int_0^s -\Sigma(X(\tau), \Omega(\tau), E(\tau))d\tau}
 \end{aligned}
 \tag{149}$$

where C_1, \dots, C_5 are some constants.

Taking into account the conditions in (147), we see that the solution (the characteristics) of the augmented system must satisfy the initial condition of the form

$$\begin{aligned}
 (X(0), \Omega(0), \mathcal{E}(0), T(0), U(0)) &= (x', \omega, E, 0), \quad t' = 0 \\
 (X(0), \Omega(0), \mathcal{E}(0), T(0), U(0)) &= (h(v), \omega, E, t', g(h(v), \omega, E, t')), \quad t' > 0
 \end{aligned}
 \tag{150}$$

where $h = h(v)$ is a local parametrization of ∂G . Also, x (resp. t) was replaced by x' (resp. t') for notational reasons. Matching the initial condition (150) to the solution (149) we get the solution $(X(s), \Omega(s), \mathcal{E}(s), T(s), \Psi(s))$ and by eliminating x', v, t', ω, E from the system

$$(X(s), \Omega(s), \mathcal{E}(s), T(s)) = (x, \omega, E, t)$$

and noting that for $t' > 0$ (formally)

$$\Psi(s) = H(t')g(x - s\omega, \omega, E, t')e^{\int_0^s -\Sigma(x - \tau\omega, \omega, E)d\tau}, \quad \text{with } s = t(x, \omega),$$

we get the solution u as in section 3.3. The result is

$$\begin{aligned}
 u(x, \omega, E, t) &= H\left(t - \sqrt{\frac{m}{2E}}t(x, \omega)\right) g\left(x - t(x, \omega)\omega, \omega, E, t - \sqrt{\frac{m}{2E}}t(x, \omega)\right) e^{\int_0^{t(x, \omega)} -\Sigma(x - \tau\omega, \omega, E)d\tau}.
 \end{aligned}
 \tag{151}$$

where H is again the Heaviside function.

For three particles system the solution is (when $E > 0$)

$$u(x, \omega, E, t) = (u_1(x, \omega, E, t), u_2(x, \omega, E, t), u_3(x, \omega, E, t))$$

where

$$\begin{aligned}
 u_j(x, \omega, E, t) &= H\left(t - \sqrt{\frac{m_j}{2E}}t(x, \omega)\right) g_j\left(x - t(x, \omega)\omega, \omega, E, t - \sqrt{\frac{m_j}{2E}}t(x, \omega)\right) e^{\int_0^{t(x, \omega)} -\Sigma_j(x - \tau\omega, \omega, E)d\tau}.
 \end{aligned}
 \tag{152}$$

Let $w = \psi - u$. Then we find that

$$(153) \quad \frac{\partial w}{\partial t} - \tilde{\mathbf{A}}w + \tilde{\Sigma}w - \tilde{K}w = \tilde{f} - \left(\frac{\partial u}{\partial t} - \tilde{\mathbf{A}}u + \tilde{\Sigma}u\right) + \tilde{K}u = \tilde{f} + \tilde{K}u \geq 0$$

$$(154) \quad w|_{\Gamma_- \times [0, T]} = g - g = 0$$

$$(155) \quad w(0) = \psi(0) - u(0) = \psi_0 \geq 0.$$

Notice that here $\psi_0|_{\Gamma_-}$ is not necessarily zero (that is, the compatibility condition is not necessarily true) and that $\tilde{f} + \tilde{K}u$ does not necessarily belong to the space $C^1([0, T], L^1(G \times S \times I)^3)$. The solution can be understood in the mild sense, although we omit the treatment of these details here; see e.g. [21] Section VI.7.a, or [42], p. 106. Hence by part A. of the proof, $w \geq 0$ and hence $\psi = w + u \geq 0$ which completes the proof. \square

6.1. A Note on Regularity of Solutions. Above given existence results of solutions for the coupled system can be analogously obtained also for general $p \in [1, \infty[$. For $p > 1$ one needs the both conditions (68), (69) and also (77), (78) of the cross-sections. In [51] (see also [9]) we have shown the dissipativity of the scattering-collision operator and related existence results (for the stationary problem) of coupled system in the case $p = 2$ by applying so-called *Lions-Lax-Milgram Theorem* (generalized Lax Milgram Theorem) ([26], Lemma 4.4.4.1, p. 234). This approach offers for $p = 2$ an alternative method. We also point out that the dimension n of the Euclidean space \mathbb{R}^n can be any $n \geq 1$ (i.e. not only $n = 3$). We omit these generalizations in this paper.

Let $m = (m_1, m_2, m_3) \in \mathbb{N}_0^3$ be a multi-index and let $U \subset G \times S \times I$ be an open subset. Define Sobolev spaces $H^{p,m}(U)$ (formally) by

$$H^{p,m}(U) = \{\psi \in L^p(G \times S \times I) \mid \partial_x^\alpha \partial_\omega^\beta \partial_E^\gamma \psi \in L^p(U), \forall |\alpha| \leq m_1, |\beta| \leq m_2, |\gamma| \leq m_3\},$$

where the derivatives are taken in the distributional sense, and where $\tilde{\omega} = (\tilde{\omega}_1, \tilde{\omega}_2)$ is a local coordinate chart in S , and $\partial_{\tilde{\omega}_j}$, $j = 1, 2$ are the respective coordinate vector fields. The rigorous definition would involve, for example, the use of multiple local charts of S covering it, along with an associated partition of unity, or the use of covariant derivatives with respect to the Levi-Civita connection on S (cf. [30] for this latter point of view). We ignore, however, these minor technicalities here to stay brief. Spaces $H^{p,m}(U)$ are mixed-norm Sobolev spaces. They are Banach spaces when equipped with the respective norms

$$\|\psi\|_{H^{p,m}(U)} = \sum_{|\alpha| \leq m_1} \sum_{|\beta| \leq m_2} \sum_{|\gamma| \leq m_3} \|\partial_x^\alpha \partial_\omega^\beta \partial_E^\gamma \psi\|_{L^p(U)}.$$

The spaces $H^{p,m}(\Gamma_-)$ can be defined in similar fashion. Finally one defines

$$W^{p,m}(U) = \{\psi \in H^{p,m}(U) \mid \omega \cdot \nabla_x \psi \in H^{p,m}(U)\}$$

These mixed-norm Sobolev spaces could be replaced by mixed-norm Bessel potential spaces or Sobolev spaces with fractional index s (so-called Slobodeckij spaces, cf. [41]). Then the multi-index m is replaced by the tuple $s = (s_1, s_2, s_3) \in \mathbb{R}_+^3$. Above $p \in [1, \infty[$ is the Lebesgue index and s is the regularity index indicating how "smooth" the functions f and g are (the tuple s refer to the orders of the distributional derivatives of the functions of spaces under consideration).

A natural question one can, and should, pose is the following: What can be said about the regularity of a solution of the equation

$$\begin{aligned} (-\mathbf{A} + \Sigma - K)\psi &= f, \\ \psi|_{\Gamma_-} &= g, \end{aligned}$$

when the cross-sections Σ_j , σ_{jk} and the data f and g are sufficiently regular, say $f \in H^{p,s}(G \times S \times I)^3$ and $g \in H^{p,s'}(\Gamma_-)^3$? Is it possible to conclude that $\psi \in W^{p',s''}(U)^3$, for some indexes p' , s'' and some open subset U of $G \times S \times I$?

In addition, the same kind of questions can be formulated for time-dependent problems. One possibility in both of these stationary and time-dependent problems for systematic study is to apply the extensive theory of pseudo-differential and especially singular integral operator theory (cf. [32]).

The regularity results are important among others in the connection of numerical methods, for example in the case when one applies higher order spline approximations (to get more rapid convergence results).

For monokinetic (one-velocity), one particle transport equations some regularity results can be found in [5] (Chapter 4, see also the introduction of the monograph for related literature). Regularity results therein are concerning for periodic solutions, solutions for so called plane-parallel problems and for problems in three-dimensional domain G . Typically the increment of regularity is "small" (only of order ≤ 1). The formulations are exhibited with the help of appropriate difference-differential norms (and the corresponding spaces), which are closely related to (or are the same as) the Bessel potential and/or Sobolev-Sobolev spaces.

The following example shows that in the case of transport equations, the regularity of the solution *does not generally* arise from the regularity of data and cross-sections in the sense that "the solution is more and more regular on the whole domain $G \times S \times I$ when the data and cross-sections are more and more regular".

Example 6.4 Let $G = B(0, r) \subset \mathbb{R}^3$ and consider the problem (for one particle)

$$\begin{aligned} \omega \cdot \nabla \psi + \psi &= 1, \\ \psi|_{\Gamma_-} &= 0. \end{aligned}$$

By (38) the solution of the problem is

$$\psi = 1 - e^{-t(x, \omega)},$$

where, by virtue of Example 3.1

$$t(x, \omega) = \langle x, \omega \rangle + \sqrt{\langle x, \omega \rangle^2 + r^2 - \|x\|^2}.$$

Here $\Sigma = 1$, $K = 0$, $f = 1 \in H^{(p, (\infty, \infty, \infty))}(G \times S \times I)$ and $g = 0 \in H^{(p, (\infty, \infty, \infty))}(\Gamma_-)$.

We see that $\psi \in C^\infty(G \times S \times I)$ since $r^2 - \|x\|^2 > 0$ for $x \in G$. Hence $\psi \in H^{(p, (\infty, \infty, \infty))}(U)$ for any subset $U \subset G \times S \times I$ which is of the form $U = G' \times S \times I$ where $G' \subset G$ is open such that $\overline{G'} \subset G$. In particular, $\psi \in H^{(p, (\infty, \infty, \infty))}(U_\epsilon)$ for any $U_\epsilon := G_\epsilon \times S \times I$ where $G_\epsilon := B(0, r - \epsilon) = \{x \in G \mid d(x, \partial G) > \epsilon\}$.

We show that $\psi \in H^{(p, (1, 0, 0))}(G \times S \times I)$ for any $1 \leq p \leq 2$ but $\psi \notin H^{(p, (1, 0, 0))}(G \times S \times I)$ for any $p \geq 3$.

Let $p \geq 1$. Since ψ is independent of E and since I is bounded we can leave E away and consider computations in spaces $H^{(p, (1, 0, 0))}(G \times S)$ only. We find that

$$\frac{\partial \psi}{\partial x_j} = e^{-t(x, \omega)} \frac{\partial t}{\partial x_j} = e^{-t(x, \omega)} \omega_j + e^{-t(x, \omega)} \frac{\langle \omega, x \rangle \omega_j - x_j}{(\langle \omega, x \rangle^2 + r^2 - \|x\|^2)^{1/2}} =: u_1 + u_2.$$

Since $e^{-2r} \leq e^{-t(x,\omega)} \leq 1$ we observe that $u_1 \in L^p(G \times S)$ and $u_2 \in L^p(G \times S)$ if and only if

$$\int_G \int_S \frac{|\langle \omega, x \rangle \omega_j - x_j|^p}{(\langle \omega, x \rangle^2 + r^2 - \|x\|^2)^{p/2}} < \infty.$$

We may compute ($p \geq 1$):

$$\begin{aligned} I_{p,j}(r) &:= \int_G \int_S \frac{|\langle \omega, x \rangle \omega_j - x_j|^p}{(\langle \omega, x \rangle^2 + r^2 - \|x\|^2)^{p/2}} d\omega dx = \int_{S \times S} \int_0^r \frac{|s \langle \omega, \lambda \rangle \omega_j - s \lambda_j|^p}{(s^2 \langle \omega, \lambda \rangle^2 + r^2 - s^2)^{p/2}} ds d\lambda d\omega \\ &= \int_{S \times S} |\langle \omega, \lambda \rangle \omega_j - \lambda_j|^p \int_0^r \frac{s^p}{(-s^2(1 - \langle \omega, \lambda \rangle^2) + r^2)^{p/2}} ds d\lambda d\omega \\ &= \int_{S \times S} |\langle \omega, \lambda \rangle \omega_j - \lambda_j|^p J_p(r; \omega, \lambda) d\lambda d\omega, \end{aligned}$$

(integrand is non-negative so one could apply Fubini's theorem in the first step) where

$$J_p(r; \omega, \lambda) = \int_0^r \frac{s^p}{(-cs^2 + r^2)^{p/2}} ds$$

and $c = c(\lambda, \omega) := 1 - \langle \omega, \lambda \rangle^2$, which belong to the interval $[0, 1]$. Thus, defining for $\tau \in [0, 1]$,

$$J_p(r; \tau) = \int_0^r \frac{s^p}{(-\tau s^2 + r^2)^{p/2}} ds,$$

we have $J_p(r, c(\omega, \lambda)) = J_p(r; \omega, \lambda)$.

Performing two consecutive changes of variables gives

$$\begin{aligned} J_p(r; \omega, \lambda) &= \int_0^r \frac{s^p}{(-cs^2 + r^2)^{p/2}} ds = \int_0^r \frac{1}{(-c + (r/s)^2)^{p/2}} ds = r \int_1^\infty \frac{1}{(-c + t^2)^{p/2} t^2} dt \\ &= \frac{r}{2} \int_1^\infty \frac{1}{(-c + v)^{p/2} v^{3/2}} dv. \end{aligned}$$

From this we see that for $0 \leq \tau < 1$, $J_p(r; \tau) < +\infty$ but $J_p(r; 1) = +\infty$.

Write for $\omega \in S$ and $a, b \in]0, 1[$, $a < b$,

$$(156) \quad I_{p,j}(r; \omega, a, b) = \int_{S(\omega, a, b)} |\langle \omega, \lambda \rangle \omega_j - \lambda_j|^p J_p(r; \omega, \lambda) d\lambda,$$

$$(157) \quad S(\omega, a, b) := \{\lambda \in S \mid a < c(\omega, \lambda) < b\}.$$

Then we have (recall that $J_p(r; \omega, \lambda) \geq 0$)

$$\int_S |\langle \omega, \lambda \rangle \omega_j - \lambda_j|^p J_p(r; \omega, \lambda) d\lambda = I_{p,j}(r; \omega, 0, 1/2) + I_{p,j}(r; \omega, 1/2, 1),$$

because the sets $\{\lambda \in S \mid c(\omega, \lambda) = \tau\}$ for $\tau \in \{0, 1/2, 1\}$ have measure zero in S .

We will first study $I_{p,j}(r; \omega, 0, 1/2)$. If $0 < c < 1/2$, and $s \in [0, r]$ we have $-cs^2 + r^2 \geq -s^2/2 + r^2 > 0$ and thus

$$J_p(r; \omega, \lambda) \leq \int_0^r \frac{s^p}{(-s^2/2 + r^2)^{p/2}} ds = J_p(r; 1/2) < \infty,$$

which allows us to estimate

$$\begin{aligned} I_{p,j}(r; \omega, 0, 1/2) &\leq J_p(r; 1/2) \int_{S(\omega, 0, 1/2)} |\langle \omega, \lambda \rangle \omega_j - \lambda_j|^p d\lambda \\ &\leq J_p(r; 1/2) \int_{S(\omega, 0, 1/2)} (|\langle \omega, \lambda \rangle| |\omega_j| + |\lambda_j|)^p d\lambda \\ &\leq 2^p J_p(r; 1/2) |S(\omega, 0, 1/2)| = 2^p J(r; 1/2) |S(e_3, 0, 1/2)|, \end{aligned}$$

where we used the $SO(3)$ -invariance of the measure on S : Given $\omega \in S$, let $M \in SO(3)$ be such that $Me_3 = \omega$, then (notice that $c(\omega, M^{-1}\lambda) = c(M\omega, \lambda) = c(e_3, \lambda)$)

$$\begin{aligned} |S(\omega, 0, \tau)| &= \int_S \chi_{S(\omega, 0, \tau)}(\lambda) d\lambda = \int_S \chi_{S(\omega, 0, \tau)}(M\lambda) d\lambda = \int_S \chi_{S(M^{-1}\omega, 0, \tau)}(\lambda) d\lambda \\ &= \int_S \chi_{S(e_3, 0, \tau)}(\lambda) d\lambda = |S(e_3, 0, \tau)|. \end{aligned}$$

Hence the above shows that for all $\omega \in S$,

$$I_{p,j}(r; \omega, 0, 1/2) \leq 2^p J_p(r; 1/2) |S(e_3, 0, 1/2)|,$$

which implies that

$$(158) \quad \int_S I_{p,j}(r; \omega, 0, 1/2) d\omega \leq 2^p J_p(r; 1/2) |S(e_3, 0, 1/2)| |S| < \infty.$$

We are now left with the task of studying $I_{p,j}(r; \omega, 1/2, 1)$ and its integral over S . If $1/2 < c < 1$ and $v \geq 2$, then $v \geq v - c \geq 1$ and

$$\frac{1}{v^{(p+3)/2}} \leq \frac{1}{(-c + v)^{p/2} v^{3/2}} \leq \frac{1}{v^{3/2}},$$

hence

$$K_p \leq J_p(r; \omega, \lambda) - \frac{r}{2} \int_1^2 \frac{1}{(-c + v)^{p/2} v^{3/2}} dv \leq K_0,$$

where

$$K_t = \int_2^\infty \frac{1}{v^{(t+3)/2}} dv < \infty, \quad t \geq 0.$$

Thus, because

$$\int_S \int_{S(\omega, 1/2, 1)} |\langle \omega, \lambda \rangle \omega_j - \lambda_j|^p K_t d\lambda d\omega < \infty$$

for all $t \geq 0$, we are only concerned with the convergence, or the divergence, of

$$(159) \quad \int_S \int_{S(\omega, 1/2, 1)} |\langle \omega, \lambda \rangle \omega_j - \lambda_j|^p J'_p(c(\omega, \lambda)) d\lambda d\omega,$$

where (note that we drop here the irrelevant factor $r/2$ in front of the integral),

$$J'_p(\tau) := \int_1^2 \frac{1}{(-\tau + v)^{p/2} v^{3/2}} dv, \quad 0 < \tau < 1.$$

But as $v \in [1, 2]$ in the domain of integration, we have

$$(160) \quad \frac{1}{2^{3/2}} \int_1^2 \frac{1}{(-\tau + v)^{p/2}} dv \leq J'_p(\tau) \leq \int_1^2 \frac{1}{(-\tau + v)^{p/2}} dv,$$

and because for $0 < \tau < 1$, and $p \geq 1$, $p \neq 2$,

$$\int_1^2 \frac{1}{(-\tau + v)^{p/2}} dv + \frac{2}{2-p} \cdot \frac{1}{(1-\tau)^{p/2-1}} = \frac{2}{2-p} \frac{1}{(2-\tau)^{p/2-1}}$$

and

$$\frac{2}{(2-p)2^{p/2-1}} \leq \frac{2}{2-p} \frac{1}{(2-\tau)^{p/2-1}} \leq \frac{2}{2-p}.$$

This shows that in the considerations of the convergence of (159) for $p \geq 1$, $p \neq 2$, one may replace the integral $J'_p(\tau)$ with the expression (from which we drop here the irrelevant factor $2/(2-p)$)

$$J''_p(\tau) := \frac{1}{(1-\tau)^{p/2-1}}, \quad 0 < \tau < 1.$$

We consider first for $p \neq 2$, $0 < a < b < 1$ (to be compared with (156))

$$\begin{aligned} I''_{p,j}(\omega, a, b) &:= \int_{S(\omega, a, b)} |\langle \omega, \lambda \rangle \omega_j - \lambda_j|^p J''_p(c(\omega, \lambda)) d\lambda \\ &= \int_{S(\omega, a, b)} |\langle \omega, \lambda \rangle \omega_j - \lambda_j|^p \frac{1}{(1-c(\omega, \lambda))^{p/2-1}} d\lambda \\ (161) \quad &= \int_{S(\omega, a, b)} \frac{|\langle \omega, \lambda \rangle \omega_j - \lambda_j|^p}{|\langle \omega, \lambda \rangle|^{p-2}} d\lambda \end{aligned}$$

If $p < 2$, we have

$$I''_{p,j}(\omega, 1/2, 1) \leq 2^p \int_S |\langle \omega, \lambda \rangle|^{2-p} d\lambda = 2^p \int_S |\langle e_3, \lambda \rangle|^{2-p} d\lambda$$

where in the last step we used the $SO(3)$ -invariance of the integral. This is clearly finite and therefore the same is true for

$$\int_S I''_{p,j}(\omega, 1/2, 1) d\omega \leq 2^p |S| \int_S |\langle e_3, \lambda \rangle|^{2-p} d\lambda < \infty.$$

All in all, this allows us to conclude that for $1 \leq p < 2$, the integral $I_{p,j}(r)$ converges, which is what we were set out to show.

Before going to the case $p > 2$, we show that for $p = 2$, one has $I_{2,j}(r) < \infty$ as well. Indeed, in this case (see (160))

$$\int_1^2 \frac{1}{(-\tau + u)^{p/2}} du = \int_1^2 \frac{1}{-\tau + u} du = \ln(2-\tau) - \ln(1-\tau),$$

and therefore, as $0 < \tau < 1$,

$$0 \leq \int_1^2 \frac{1}{(-\tau + u)^{p/2}} du + \ln(1-\tau) \leq \ln(2),$$

we see that it is enough to consider to show the convergence (or the divergence) of

$$I''_{2,j}(r) = \int_S \int_{S(\omega, \tau, 1)} -|\langle \omega, \lambda \rangle \omega_j - \lambda_j|^2 \ln(1-c(\omega, \lambda)) d\lambda d\omega.$$

But $\lambda \in S(\omega, 1/2, 1)$ if and only if $0 < |\langle \omega, \lambda \rangle| \leq 1/\sqrt{2}$, and because $\ln(1 - c(\omega, \lambda)) = 2 \ln |\langle \omega, \lambda \rangle|$, we have

$$\begin{aligned} I''_{2,j}(r) &\leq 8 \int_S \int_{S(\omega, 1/2, 1)} -\ln |\langle \omega, \lambda \rangle| d\lambda d\omega = 8 \int_S \int_{S(e_3, 1/2, 1)} -\ln |\langle e_3, \lambda \rangle| d\lambda d\omega \\ &= 16\pi |S| \int_{\left\{ \begin{smallmatrix} \theta \in [0, \pi] \\ 0 < |\cos(\theta)| < 1/\sqrt{2} \end{smallmatrix} \right\}} -\ln |\cos(\theta)| d\theta \\ &= 32\pi |S| \int_{\left\{ \begin{smallmatrix} \theta \in [0, \pi/2] \\ 0 < \sin(\theta) < 1/\sqrt{2} \end{smallmatrix} \right\}} -\ln(\sin(\theta)) d\theta = 32\pi |S| \int_0^{1/\sqrt{2}} \frac{-\ln(t)}{\sqrt{1-t^2}} dt \\ &\leq 32\sqrt{2}\pi |S| \int_0^{1/\sqrt{2}} -\ln(t) dt = 32\pi |S| (1 + \ln \sqrt{2}) < \infty. \end{aligned}$$

This shows that the integral $I''_{p,j}(r)$, and therefore $I_{p,j}(r)$, converges in the case $p = 2$ as well.

For the rest of the computations, we shall assume that $p > 2$. Let $\|\cdot\|_p$ denote the p -norm on \mathbb{R}^3 and let $C_p > 0$ be a constant such that $\|\cdot\|_p \geq C_p \|\cdot\|_2$ on \mathbb{R}^3 . We consider for $0 < \tau < 1$ (and take $\tau = 1/2$ eventually)

$$I''_p(\omega, \tau, 1) := \sum_{j=1}^3 I''_{p,j}(\omega, \tau, 1) = \int_{S(\omega, \tau, 1)} \frac{\|\lambda - \langle \omega, \lambda \rangle \omega\|_2^p}{|\langle \omega, \lambda \rangle|^{p-2}} d\lambda.$$

This can be estimated by below by

$$I''_p(\omega, \tau, 1) \geq C_p^p \int_{S(\omega, \tau, 1)} \frac{\|\lambda - \langle \omega, \lambda \rangle \omega\|_2^p}{|\langle \omega, \lambda \rangle|^{p-2}} d\lambda.$$

Notice that $\lambda - \langle \omega, \lambda \rangle \omega$ is orthogonal to ω and has 2-norm (Euclidean norm)

$$\|\lambda - \langle \omega, \lambda \rangle \omega\|_2^2 = 1 - \langle \omega, \lambda \rangle^2 = c(\omega, \lambda).$$

Therefore if $\lambda \in S(\omega, 1/2, 1)$ and hence $c(\omega, \lambda) > 1/2$, we can estimate

$$\begin{aligned} I''_p(\omega, \tau, 1) &\geq (C_p/\sqrt{2})^p \int_{S(\omega, \tau, 1)} \frac{1}{|\langle \omega, \lambda \rangle|^{p-2}} d\lambda = (C_p/\sqrt{2})^p \int_{S(e_3, 1/2, 1)} \frac{1}{|\langle e_3, \lambda \rangle|^{p-2}} d\lambda \\ &= 2\pi (C_p/\sqrt{2})^p \int_{\left\{ \begin{smallmatrix} \theta \in [0, \pi] \\ 0 < |\cos(\theta)| < 1/\sqrt{2} \end{smallmatrix} \right\}} \frac{1}{|\cos(\theta)|^{p-2}} d\theta \\ &= 4\pi (C_p/\sqrt{2})^p \int_{\left\{ \begin{smallmatrix} \theta \in [0, \pi/2] \\ 0 < \sin(\theta) < 1/\sqrt{2} \end{smallmatrix} \right\}} \frac{1}{|\sin(\theta)|^{p-2}} d\theta \\ &= 4\pi (C_p/\sqrt{2})^p \int_0^{1/\sqrt{2}} \frac{1}{t^{p-2} \sqrt{1-t^2}} dt \geq 4\pi (C_p \sqrt{\tau})^p \int_0^{1/\sqrt{2}} \frac{1}{t^{p-2}} dt. \end{aligned}$$

These estimates lead to the conclusion that

$$I''_p(\omega, 1/2, 1) = +\infty, \quad \forall p \geq 3,$$

and therefore $\int_S I''_p(\omega, 1/2, 1) d\omega = +\infty$ whenever $p \geq 3$. Taking into account the observations we have made previously, this shows that

$$I_p(r) := \sum_{j=1}^3 I_{p,j}(r) = +\infty, \quad \forall p \geq 3.$$

To sum up, we have shown that

$$u_2 \in L^p(G \times S) \text{ when } 1 \leq p \leq 2 \text{ and } u_2 \notin L^p(G \times S), \text{ when } p \geq 3,$$

and hence that

$$\psi \in H^{(p,(1,0,0))}(G \times S) \text{ when } 1 \leq p \leq 2 \text{ and } \psi \notin H^{(p,(1,0,0))}(G \times S), \text{ when } p \geq 3.$$

7. RELATED (OPTIMAL) CONTROL PROBLEM AND RADIATION TREATMENT PLANNING

7.1. Control Problem. In the following we let p be in the interval $[1, \infty[$ (cf. Remark 6.1). The most reasonable (and practical) choices are $p = 2$ and $p = 1$. From the control theoretic point of view a relevant output mapping for the stationary problem in radiation therapy is the dose (distribution)

$$(162) \quad D(x) := (D\psi)(x) = \sum_{j=1}^3 \int_{S \times I} \kappa_j(x, E) \psi_j(x, \omega, E) d\omega dE$$

where $\kappa_j \in L^\infty(G \times I)$, $\kappa_j \geq 0$, are the so-called *energy-deposition cross sections* ([9], [37]). We find that $D : L^p(G \times S \times I)^3 \rightarrow L^p(G)$ is a bounded linear operator and

$$(163) \quad \|D\psi\|_{L^p(G)} \leq m(G \times S \times I)^{1/p'} \left(\max_{1 \leq j \leq 3} \|\kappa_j\|_{L^\infty(G \times I)} \right) \|\psi\|_{L^p(G \times S \times I)^3}$$

where $m(G \times S \times I)$ is the measure of $G \times S \times I$ and $\frac{1}{p} + \frac{1}{p'} = 1$, with the convention that $m(G \times S \times I)^{1/p'} = 1$, if $p = 1$.

In the case of time-dependent problem the dose (distribution) is

$$(164) \quad D(x, t) := D(\psi(t))(x) = \sum_{j=1}^3 \int_{S \times I} \kappa_j(x, E) \psi_j(x, \omega, E, t) d\omega dE$$

where $D(\cdot, \cdot) \in C([0, T], L^p(G))$ (or only in $L^1([0, T], L^p(G))$). D is an operator $C([0, T], L^p(G \times S \times I)^3) \rightarrow C([0, T], L^p(G))$, and the total dose in time interval $[0, T]$ is given by

$$D(x) = (D\psi)(x) = \int_0^T D(x, t) dt.$$

7.1.1. Time-dependent Control System. The time-dependent BTE system in its abstract form for $\psi_0 = 0$ is

$$(165) \quad \frac{\partial \psi}{\partial t} - \tilde{\mathbf{A}}\psi + \tilde{\Sigma}\psi - \tilde{K}\psi = \tilde{f},$$

$$(166) \quad \psi|_{\Gamma_- \times]0, T]} = g$$

where we assume that $g(0) = 0$ (the compatibility condition). Using the lift $Lg := (Lg_1, Lg_2, Lg_3) \in C^2([0, T], \mathcal{W}^p(G \times S \times I)^3)$ as obtained analogously to Lemma 5.11, and denoting $u = \psi - Lg$ the equation (165) becomes (note that $u(t) \in \tilde{\mathcal{W}}_{-,0}^p(G \times S \times I) = D(\tilde{\mathbf{A}}_0)$)

$$(167) \quad \frac{\partial u}{\partial t} = (\tilde{\mathbf{A}}_0 - \tilde{\Sigma} + \tilde{K})u - \left(\frac{\partial}{\partial t} - \tilde{\mathbf{A}} + \tilde{\Sigma} - \tilde{K} \right) Lg + \tilde{f}$$

$$(168) \quad := \mathcal{A}_0 u + \mathcal{A}Lg - \frac{\partial(Lg)}{\partial t} + \tilde{f}$$

where $\mathcal{A} := \tilde{\mathbf{A}} - \tilde{\Sigma} + \tilde{K}$ and \mathcal{A}_0 is its restriction to $D(\mathcal{A}_0) := D(\tilde{\mathbf{A}}_0) = \tilde{\mathcal{W}}_{-,0}^p(G \times S \times I)^3$. Hence we have a relevant control system

$$(169) \quad \frac{\partial u}{\partial t} = \mathcal{A}_0 u + \mathcal{A} Lg - \frac{\partial(Lg)}{\partial t} + \tilde{f},$$

$$(170) \quad u(0) = 0$$

$$(171) \quad y = D(\psi(\cdot)) = D(u(\cdot)) + D(Lg(\cdot))$$

where we have $\frac{\partial(Lg)}{\partial t} = L \frac{\partial g}{\partial t}$ (see the proof of Lemma 5.11).

Let $T > 0$. Define

$$H_T(\tilde{f}, g) := u(T) = \int_0^T \tilde{G}(t-s) \left(\mathcal{A} Lg - \frac{\partial(Lg)}{\partial t} + \tilde{f} \right)(s) ds$$

where $\tilde{G}(t)$ is (as above) the semigroup generated by \mathcal{A}_0 . In external therapy we have $\tilde{f} = 0$ and in internal (brachy) therapy $g = 0$.

The important and relevant problems are the following ones. Let $T > 0$ and let $\mathcal{C} := \{g \in C^2([0, T], \mathcal{T}^p(\Gamma_-)^3) \mid g(0) = 0, g \geq 0\}$ and $\mathcal{C}' = \{\tilde{f} \in C^1([0, T], L^p(G \times S \times I)^3) \mid \tilde{f} \geq 0\}$. How to characterize the sets

$$\mathcal{S}_T := \{H_T(0, g) = \psi(T) = u(T) + (Lg)(T) \mid g \in \mathcal{C}\} \subset L^p(G \times S \times I)^3$$

and

$$\mathcal{S}'_T := \{H_T(\tilde{f}, 0) = \psi(T) \mid \tilde{f} \in \mathcal{C}'\} \subset L^p(G \times S \times I)^3$$

that is, *what are the possible states $\psi(T)$ that can be produced using the controls chosen from \mathcal{C} and \mathcal{C}' , respectively, during the time T ?* Similarly for the doses: What can be said about the sets

$$\mathcal{D}_T := \{y = D(\psi(T)) \mid g \in \mathcal{C}\} \subset L^p(G).$$

and

$$\mathcal{D}'_T := \{y = D(\psi(T)) \mid \tilde{f} \in \mathcal{C}'\} \subset L^p(G).$$

that is, *which are the dose distributions D that one can produce using the controls chosen from \mathcal{C} and \mathcal{C}' , respectively, during the time T ?* Here \mathcal{C} may be replaced with a larger space such as with $\{g \in H^1([0, T], \mathcal{T}^p(\Gamma_-)^3) \mid g(0) = 0, g \geq 0\}$. Similarly, \mathcal{C}' can be replaced e.g. with the set $\{\tilde{f} \in H^1([0, T], L^p(G \times S \times I)^3) \mid \tilde{f} \geq 0\}$.

Similarly for the total doses we can impose the problem: What can be said about the sets

$$\mathcal{D} := \{y = D\psi \mid g \in \mathcal{C}\} \subset L^p(G)$$

and

$$\mathcal{D}' := \{y = D\psi \mid \tilde{f} \in \mathcal{C}'\} \subset L^p(G)$$

that is, *which are the total dose distributions that one can produce using controls chosen from \mathcal{C} and \mathcal{C}' , respectively, during the time T ?*

It has been shown that in a certain simplified case for one particle there exists $T > 0$ such that $\mathcal{S}_T = L^p(G \times S \times I)$ for $p = 2$ ([2]), which means that the control system is *exactly controllable*. For a general background on infinite dimensional control systems and related concepts, we refer to [17], [53]. Note that in the above control problem, the time derivative of the control g appears in the system which makes the problem more nonstandard.

Remark 7.1 The control system (169) can be written in the form

$$\dot{u} = \mathcal{A}_0 u + \mathcal{B}v + \mathcal{C}\dot{v}$$

where $v := (\tilde{f}, g)$ (the control variable) and

$$\begin{aligned} \mathcal{A}_0 &= \tilde{\mathbf{A}}_0 - \tilde{\Sigma} + \tilde{K} : L^p(G \times S \times I)^3 \rightarrow L^p(G \times S \times I)^3 \\ \mathcal{B} &= \mathcal{A} \circ L \circ \text{pr}_2 + \text{pr}_1 \\ &: L^1(G \times S \times I)^3 \times C^1([0, T], T^1(\Gamma_-)) \rightarrow C([0, T], L^1(G \times S \times I)^3) \\ \mathcal{C} &= -L \circ \text{pr}_2 \\ &: L^1(G \times S \times I)^3 \times C^1([0, T], T^1(\Gamma_-)) \rightarrow C^1([0, T], \tilde{W}^1(G \times S \times I)). \end{aligned}$$

Here pr_1, pr_2 are projections onto the first and the second factors of the cartesian product space $L^1(G \times S \times I)^3 \times C^1([0, T], T^1(\Gamma_-))$.

7.1.2. Stationary Control Problem. The corresponding control problems can also be stated for the stationary problem which we sketch as follows. The forward problem is

$$(172) \quad \begin{aligned} -\mathbf{A}\psi + \Sigma\psi - K\psi &= f, \\ \psi|_{\Gamma_-} &= g, \end{aligned}$$

where $f \in L^p(G \times S \times I)^3$, $g \in T^p(\Gamma_-)$. Using the lift $Lg := (Lg_1, Lg_2, Lg_3) \in \tilde{W}^p(G \times S \times I)^3$ and denoting $u = \psi - Lg$ the system (172) becomes

$$(173) \quad (-\mathbf{A}_0 + \Sigma - K)u = f - (-\mathbf{A} + \Sigma - K)Lg$$

where $u \in \tilde{W}_{-,0}^p(G \times S \times I)^3 = D(\mathbf{A}_0)$. Hence we have (under the assumptions of Theorem 5.6)

$$(174) \quad \begin{aligned} u &= (-\mathbf{A}_0 + \Sigma - K)^{-1}(f - (-\mathbf{A} + \Sigma - K)Lg) \\ y &= D\psi = Du + D(Lg) = D\left[(-\mathbf{A}_0 + \Sigma - K)^{-1}(f - (-\mathbf{A} + \Sigma - K)Lg)\right] + D(Lg). \end{aligned}$$

Again, the relevant problems in this stationary case are the following ones. How to characterize the sets (external therapy)

$$\mathcal{S} := \{\psi = u + Lg = -(-\mathbf{A}_0 + \Sigma - K)^{-1}(-\mathbf{A} + \Sigma - K)Lg + Lg \mid g \in T^p(\Gamma_-)^3, g \geq 0\}$$

and (internal therapy)

$$\mathcal{S}' := \{\psi = (-\mathbf{A}_0 + \Sigma - K)^{-1}f \mid f \in L^p(G \times S \times I)^3, f \geq 0\}.$$

For the dose distributions, it is important to describe the structures of the sets

$$\mathcal{D} := \{D\psi \mid \psi \in \mathcal{S}\}$$

and

$$\mathcal{D}' := \{D\psi \mid \psi \in \mathcal{S}'\}.$$

In addition to the above problems, one of the main challenges in radiation therapy is to develop methods on how the inflow flux g and/or the internal source f can be computed when an element of \mathcal{S} (resp. \mathcal{S}_T), and especially when an element of \mathcal{D} (resp. \mathcal{D}_T), is known and the same is concerning for the sets $\mathcal{S}', \mathcal{S}'_T, \mathcal{D}', \mathcal{D}'_T$. This is known as the *Inverse Planning Problem* (see e.g. [9], [48]) which we, from the mathematical point of view, shall describe briefly below. In some simple cases the inverse problem can probably be solved analytically (cf. [40], Chapter 11), but in

real situations only *optimal inflow fluxes or internal sources* can be found. The analytical solutions are valuable (even though in simplified cases) because they may greatly help the actual optimization procedure (e.g. in seeking the initial point for the global optimization) and give insight on which kind of states or dose distributions are reasonable and possible to generate.

In some cases for $p = 2$ the related stationary *optimal control* problem has, in theory, an explicit solution. This is based on the optimal control theory for equations governed by closed densely defined coercive operators in Hilbert spaces and the convexity of the objective function and admissible sets (see section 7.2.3 and [22], [51]). The explicit solution obtained in this way can be used as an initial solution for the chosen optimization algorithm but it is not generally a ready treatment plan. The same observations remain valid for the time-dependent case. We emphasize that time-dependent models are still not (at least extensively) applied in radiation therapy. For a more extensive background of optimal control problems governed by partial differential/boundary value operators we refer to [36].

7.2. Radiation Treatment Planning. We consider here only the treatment planning based on stationary Boltzmann transport equation. Not all the configurations are achievable as dose distributions, in the sense that in general $\mathcal{D} \neq L^p(G)$, and therefore hence one can only hope to seek dose distributions which are as optimal as possible with respect to the given configuration.

7.2.1. Background. As mentioned in the introduction, radiation therapy aims to generate dose distributions in such a way that the desired dose conforms to the target volume, while the healthy tissue and especially the so-called critical organs achieve as low dose as possible. Dose can be delivered externally (external therapy) or internally (internal therapy or brachytherapy). The determination of (optimal) incoming external particle fluxes through the patches of patient surface or internal sources located inside the patient tissue is the basic task in treatment planning known as the *inverse treatment planning*.

Recall that the patient domain $G \subset \mathbb{R}^3$ consists of the tumor volume \mathbf{T} , the critical organ region \mathbf{C} and the normal tissue region \mathbf{N} , as a mutually disjoint union $G = \mathbf{T} \cup \mathbf{C} \cup \mathbf{N}$. We assume that the sets \mathbf{T} , \mathbf{C} , \mathbf{N} are Lebesgue measurable. The tumor volume, that is the target, includes the tumor and some safety margin around it. Critical organs and normal tissue are build up of healthy tissue, and must be conserved during the treatment as well as possible.

In the sequel we only deal with the inverse treatment planning problem in the context of the stationary Boltzmann transport equation (i.e. we omit time dependency here which could be treated analogously after some modifications). The dose is computed from the generated particle flux $\psi \in L^p(G \times S \times I)^3$ (as mentioned above) by

$$D(x) = (D\psi)(x) = \sum_{j=1}^3 \int_{S \times I} \kappa_j(x, E) \psi_j(x, \omega, E) d\omega dE$$

where $\psi = (\psi_1, \psi_2, \psi_3) \in L^p(G \times S \times I)^3 \subset L^1(G \times S \times I)^3$ satisfies the Boltzmann transport equation,

$$(175) \quad \begin{aligned} \omega \cdot \nabla \psi_j + \Sigma \psi_j - K\psi &= f_j \\ \psi_j|_{\Gamma_-} &= g_j, \end{aligned}$$

for $j = 1, 2, 3$, or, more shortly,

$$(176) \quad \begin{aligned} (-\mathbf{A}_0 + \Sigma - K)\psi &= f, \\ \psi|_{\Gamma_-} &= g. \end{aligned}$$

In practice g is non-zero only on a finite number of patches on patient's surface. Let $\psi = \psi(f, g)$ be the unique solution of (176) that is, as discussed in section 5.3 (under the relevant assumptions stated there)

$$(177) \quad \psi = \psi(f, g) = (-\mathbf{A}_0 + \Sigma - K)^{-1}(f - (-\mathbf{A} + \Sigma - K)Lg) + Lg.$$

The generated dose is then

$$D = D(x) = (D(\psi(f, g)))(x), \quad x \in G.$$

We denote $\mathcal{D}(f, g) := D(\psi(f, g))$. Then we have

Lemma 7.2 The dose operator $\mathcal{D} : L^p(G \times S \times I)^3 \times T^p(\Gamma_-)^3 \rightarrow L^p(G)$ is linear and bounded, i.e.

$$\|\mathcal{D}(f, g)\|_{L^p(G)} \leq C (\|f\|_{L^p(G \times S \times I)^3} + \|g\|_{T^p(\Gamma_-)^3}).$$

Proof. The following proof is complete only for $p = 1$ and $p = 2$ because (79) (and its consequence (85)) has been shown only for these cases (see Theorems 5.3 and 5.6 above, and [51]). By (174)

$$\mathcal{D}(f, g) = D \left[(-\mathbf{A}_0 + \Sigma - K)^{-1}(f - (-\mathbf{A} + \Sigma - K)Lg) \right] + D(Lg).$$

Hence \mathcal{D} is a linear operator. We show that it is bounded. Writing $C_0 := m(G \times S \times I)^{1/p'} \left(\max_{1 \leq j \leq 3} \|\kappa_j\|_{L^\infty(G \times I)} \right)$, we have by (163),

$$\begin{aligned} \|D\psi\|_{L^p(G)} &\leq C_0 \|(-\mathbf{A}_0 + \Sigma - K)^{-1}(f - (-\mathbf{A} + \Sigma - K)Lg) + Lg\|_{L^p(G \times S \times I)^3}, \\ \|D(Lg)\|_{L^p(G)} &\leq C_0 \|Lg\|_{L^p(G \times S \times I)^3}. \end{aligned}$$

Then by (85), (88), Lemma 5.8 and since $\mathbf{A}(Lg) = 0$ (as shown in the proof of the lemma)

$$\begin{aligned} \|D\psi\|_{L^p(G)} &\leq C_0 \left(\|(-\mathbf{A}_0 + \Sigma - K)^{-1}f\|_{L^p(G \times S \times I)^3} \right. \\ &\quad \left. + \|(-\mathbf{A}_0 + \Sigma - K)^{-1}(-\mathbf{A} + \Sigma - K)Lg\|_{L^p(G \times S \times I)^3} + \|Lg\|_{L^p(G \times S \times I)^3} \right) \\ &\leq C_0 \left(\frac{1}{c} \|f\|_{L^p(G \times S \times I)^3} + \frac{1}{c} \|(-\mathbf{A} + \Sigma - K)Lg\|_{L^p(G \times S \times I)^3} + \|Lg\|_{L^p(G \times S \times I)^3} \right) \\ (178) \quad &\leq C_0 \left(\frac{1}{c} \|f\|_{L^p(G \times S \times I)^3} + \frac{d}{c} \|\Sigma - K\| \|g\|_{T^p(\Gamma_-)^3} + d \|g\|_{T^p(\Gamma_-)^3} \right), \end{aligned}$$

which implies the boundedness of \mathcal{D} . □

Commonly used *physical criteria* are the following ones. We demand that

$$(179) \quad D(x) = D_0, \quad x \in \mathbf{T},$$

$$(180) \quad D(x) \leq D_C, \quad x \in \mathbf{C},$$

$$(181) \quad D(x) \leq D_N, \quad x \in \mathbf{N},$$

where D_0 is the prescribed (usually uniform) dose in target \mathbf{T} and where D_C and D_N are the allowed upper bounds in the critical organ \mathbf{C} and normal tissue \mathbf{N} regions,

respectively. Instead of (179) one may ask for more flexibly (when considering the so-called feasible solutions) that only

$$(182) \quad d_T \leq D(x) \leq D_T, \quad x \in \mathbf{T},$$

where D_T and d_T are upper and lower bounds for dose in target.

In addition to the above requirements in modern planning, one imposes so-called *dose volume constraints* for the dose distribution, especially for the critical organ region (but also for some other tissue region's similar dose volume constraints may be considered). Dose volume constraint demands that the dose $D(x)$ cannot be greater than some prescribed dose level, say d_C , in a volume fraction v_C of \mathbf{C} which is greater than some given fraction v_C . This can be expressed as follows

$$(183) \quad \frac{\mathcal{L}^3(\{x \in \mathbf{C} \mid D(x) \geq d_C\})}{\mathcal{L}^3(\mathbf{C})} \leq v_C$$

where \mathcal{L}^3 is the 3-dimensional Lebesgue measure. Clearly the dose volume constraint is equivalent to

$$(184) \quad \frac{1}{\mathcal{L}^3(\mathbf{C})} \int_{\mathbf{C}} H(D(x) - d_C) dx \leq v_C$$

where H is the Heaviside function. Note that the integral in (184) exists. In practice H can be replaced here with a smooth (or continuous) function H_ϵ which approximates it to some reasonable level of accuracy.

7.2.2. Object Function and the Optimization Problem. Our aim is that the above requirements (179), (180), (181), (183) for the dose distribution are valid as well as possible. For that purpose, we define the object (cost) function

$$(185) \quad J(f, g) = c_{\mathbf{T}} J_{\mathbf{T}}(f, g) + c_{\mathbf{C}} J_{\mathbf{C}}(f, g) + c_{\mathbf{N}} J_{\mathbf{N}}(f, g) + c_{\text{DV}} J_{\text{DV}}(f, g),$$

where

$$\begin{aligned} J_{\mathbf{T}}(f, g) &= \|D_0 - \mathcal{D}(f, g)\|_{L^p(\mathbf{T})}^p, \\ J_{\mathbf{C}}(f, g) &= \|(D_C - \mathcal{D}(f, g))_-\|_{L^p(\mathbf{C})}^p, \\ J_{\mathbf{N}}(f, g) &= \|(D_N - \mathcal{D}(f, g))_-\|_{L^p(\mathbf{N})}^p, \\ J_{\text{DV}}(f, g) &= \left(\left(v_C - \frac{1}{\mathcal{L}^3(\mathbf{C})} \int_{\mathbf{C}} H(\mathcal{D}(f, g)(x) - d_C) dx \right)_- \right)^p, \end{aligned}$$

and where $c_{\mathbf{T}}, c_{\mathbf{C}}, c_{\mathbf{N}}, c_{\text{DV}}$ are non-negative weights with which one controls the different priorities in the optimization. Here a_- denotes the negative part $\frac{1}{2}(|a| - a)$ of $a \in \mathbb{R}$. Also, notice that $J_{\text{DV}}(f, g) \leq 1$.

As mentioned above in external radiotherapy $f = 0$ and in internal radiotherapy $g = 0$ (from the mathematical point of view both can, of course, be non-zero). Thus the corresponding object functions in practice are

$$\begin{aligned} J_{\text{ex}}(g) &:= J(0, g) \quad (\text{external radiotherapy}) \text{ and} \\ J_{\text{in}}(f) &:= J(f, 0) \quad (\text{internal radiotherapy}). \end{aligned}$$

The *admissible sets* for the optimal control problems are respectively

$$U_{\text{ad}} = \{g \in T^p(\Gamma_-)^3 \mid g \geq 0\} \quad (\text{external radiotherapy})$$

and

$$U'_{\text{ad}} = \{f \in L^p(G \times S \times I)^3 \mid f \geq 0\} \quad (\text{internal radiotherapy}).$$

They both are convex sets (cones) of the ambient spaces. If (in practical optimization) one wants to take the whole ambient space as an admissible set that is, $U_{\text{ad}} = T^p(\Gamma_-)^3$ or respectively $U'_{\text{ad}} = L^p(G \times S \times I)^3$ one must add to the object function the penalty term

$$+c_{\text{ad}}J_{\text{ad}}(g), \text{ where, } J_{\text{ad}}(g) = \|g-\|_{T^p(\Gamma_-)^3}^p \text{ (external radiotherapy)}$$

and

$$+c_{\text{ad}'}J_{\text{ad}'}(f), \text{ where } J_{\text{ad}'}(f) = \|f-\|_{L^p(G \times S \times I)^3}^p \text{ (internal radiotherapy)}.$$

These take care of the non-negativity of the incoming flux or source, respectively. In theory as well as in practice, it is also reasonable to add a stabilizing cost terms correspondingly

$$(186) \quad +c_{\text{sc}}J_{\text{sc}}(g) \text{ where } J_{\text{sc}}(g) = \|\psi(0, g)\|_{L^p(G \times S \times I)^3}^p,$$

or

$$(187) \quad +c_{\text{sc}'}J_{\text{sc}'}(f) \text{ where } J_{\text{sc}'}(f) = \|\psi(f, 0)\|_{L^p(G \times S \times I)^3}^p.$$

As a conclusion, we have for the external therapy the object function

$$(188) \quad J_{\text{ex}}(g) = c_{\mathbf{T}}J_{\mathbf{T}}(0, g) + c_{\mathbf{C}}J_{\mathbf{C}}(0, g) + c_{\mathbf{N}}J_{\mathbf{N}}(0, g) + c_{\text{DV}}J_{\text{DV}}(0, g) + c_{\text{sc}}J_{\text{sc}}(g),$$

when $U_{\text{ad}} = \{g \in T^p(\Gamma_-)^3 \mid g \geq 0\}$ or

$$(189) \quad J_{\text{ex}}(g) = c_{\mathbf{T}}J_{\mathbf{T}}(0, g) + c_{\mathbf{C}}J_{\mathbf{C}}(0, g) + c_{\mathbf{N}}J_{\mathbf{N}}(0, g) + c_{\text{DV}}J_{\text{DV}}(0, g) + c_{\text{ad}}J_{\text{ad}}(g) + c_{\text{sc}}J_{\text{sc}}(g).$$

when $U_{\text{ad}} = T^p(\Gamma_-)^3$. The object function $J_{\text{in}}(f)$ for the internal therapy is formulated analogously. In practice one may have $p = 1$, which is from the physical point of view a reasonable choice, or $p = 2$, which gives mathematically a very convenient setting because of Hilbert space structure of the underlying spaces.

With these concepts the overall optimal control (boundary value problem) can be stated as : Find the *global minimum*

$$(190) \quad \min\{J_{\text{ex}}(g) \mid g \in U_{\text{ad}}\} \text{ (external radiotherapy),}$$

or

$$(191) \quad \min\{J_{\text{in}}(f) \mid f \in U_{\text{ad}}\} \text{ (internal radiotherapy),}$$

where U_{ad} or U'_{ad} , respectively, is chosen in the way explained above.

Suppose that X is a vector space and that $F : U \rightarrow \mathbb{R}$ is a function defined on a convex set $U \subset X$. We say that F is *convex* if for any choice of $x, y \in U$ it holds that

$$F(tx + (1-t)y) \leq tF(x) + (1-t)F(y), \quad 0 \leq t \leq 1.$$

F is called strictly convex if for $x, y \in U$, $x \neq y$

$$F(tx + (1-t)y) < tF(x) + (1-t)F(y), \quad 0 < t < 1.$$

Let $F_- : \mathbb{R} \rightarrow \mathbb{R}$ be the negative part function $F_-(x) = \frac{1}{2}(|x| - x)$. We find that it is non-differentiable (at $x = 0$). Hence in general case (one can show) the object functions J_{ex} and J_{in} are also non-differentiable in the (interior of the) corresponding admissible sets. However, we have for J_{ex} and J_{in} the following.

Theorem 7.3 (i) The terms

$$J_{\mathbf{T}}(0, g), J_{\mathbf{C}}(0, g), J_{\mathbf{N}}(0, g), J_{\text{ad}}(g) \text{ and } J_{\text{sc}}(g)$$

of the object function $J_{\text{ex}} : T^p(\Gamma_-)^3 \rightarrow \mathbb{R}$ are convex, and they are locally (resp. globally) Lipschitz continuous if $p \in]1, \infty[$ (resp. $p = 1$). In addition, the term

$$J_{\text{DV}}(0, g)$$

is Lipschitz continuous, if the Heaviside function H in its definition is replaced by a Lipschitz continuous approximation H_ϵ (see (233)).

(ii) When $p = 2$, the terms

$$J_{\mathbf{T}}(0, g), J_{\text{sc}}(g)$$

of the object function J_{ex} are differentiable on $T^2(\Gamma_-)^3$.

Analogous results hold for the terms of the object function J_{in} .

Proof. (i) We first show the stated convexity properties.

Recall that $\mathcal{D} : L^p(G \times S \times I)^3 \times T^p(\Gamma_-)^3 \rightarrow L^p(G)$ is linear and bounded, and hence the mapping $g \rightarrow D_0 - \mathcal{D}(0, g)$ is affine. Moreover, it is a basic fact that the map $\|\cdot\|_{L^p}^p : L^p(\mathbf{T}) \rightarrow \mathbb{R}; u \mapsto \|u\|_{L^p(\mathbf{T})}^p$ is strictly convex if $p \in]1, \infty[$ and convex if $p = 1$ (the point being that $\mathbb{R} \rightarrow \mathbb{R}; x \mapsto |x|^p$ is strictly convex, or convex, in the respective two situations). Therefore, as the composition of these two maps $J_{\mathbf{T}}(0, g)$ is clearly convex if $p \in [1, \infty[$.

To see that $J_{\mathbf{C}}(0, g), J_{\mathbf{N}}(0, g), J_{\text{ad}}(g)$ are convex, it is enough to observe that $g \rightarrow D_0 - \mathcal{D}(0, g)$ is affine, the negative part function $x \mapsto x_- = \frac{1}{2}(|x| - x)$ is convex, the map $x \mapsto x^p$ for $p \geq 1$ is increasing for $x \geq 0$ and that the integral $\int L^p(X) \rightarrow \mathbb{R}; u \mapsto \int_X u$ is linear, where X is one of the sets \mathbf{C}, \mathbf{N} or Γ_- .

Finally, $J_{\text{sc}}(g)$ is convex if $p \in [1, \infty[$, as the mapping $g \mapsto \psi(0, g)$ is linear and $u \mapsto \|u\|_{L^p(G \times S \times I)}$ is convex, in the corresponding cases.

We then move to showing the claims concerning the Lipschitz continuities of the terms of J_{ex} .

That $J_{\mathbf{T}}(0, g), J_{\mathbf{C}}(0, g), J_{\mathbf{N}}(0, g), J_{\text{ad}}(g)$ and $J_{\text{sc}}(g)$ are Lipschitz continuous (locally or globally), can be seen as follows.

By the proof of Lemma 7.2 the operator $T^p(\Gamma_-)^3 \rightarrow L^p(G \times S \times I)^3; g \mapsto \psi(0, g)$, whose value can be written as (see (177))

$$\psi(0, g) = -(-\mathbf{A}_0 + \Sigma - K)^{-1}(-\mathbf{A} + \Sigma - K)Lg + Lg$$

is linear and bounded, hence globally Lipschitz. Similarly, as the map $T^p(\Gamma_-)^3 \rightarrow L^p(G); \mathcal{D}g = \mathcal{D}(0, g)$ is linear and bounded, for any $D \in \mathbb{R}$ the affine map $g \mapsto D - \mathcal{D}(0, g)$ is globally Lipschitz.

The negative part map $\mathbb{R} \rightarrow \mathbb{R}; x \mapsto \frac{1}{2}(|x| - x)$ is globally Lipschitz, as is the norm map $u \mapsto \|u\|_{L^p(X)}$ for any $p \geq 1$, where X here is one of the sets $\mathbf{T}, \mathbf{C}, \mathbf{N}$ or Γ_- . Finally $x \mapsto x^p, x \geq 0$, is locally Lipschitz if $p > 1$ and globally Lipschitz if $p = 1$. Therefore, because $J_{\mathbf{T}}(0, g), J_{\mathbf{C}}(0, g), J_{\mathbf{N}}(0, g), J_{\text{ad}}(g)$ are appropriate composition maps of the above ones, we see that they all are locally Lipschitz when $p \in]1, \infty[$, and globally Lipschitz when $p = 1$.

Finally, noticing that $|x^p - y^p| \leq p|x - y|$ for all $x, y \in [0, 1]$, and that

$$0 \leq \left(v_C - \frac{1}{\mathcal{L}^3(\mathbf{C})} \int_{\mathbf{C}} H_\epsilon(\mathcal{D}(0, g)(x) - d_C) dx \right)_- \leq 1$$

the claimed Lipschitz continuity of $J_{\text{DV}}(0, g)$ can be established.

(ii) For $p = 2$, as $g \mapsto \psi(0, g)$, $\mathcal{D}(0, g)$ are continuous (hence smooth) linear maps, and the squared norms $\|\cdot\|_{L^2(\mathbf{T})}^2$, $\|\cdot\|_{L^2(G \times S \times I)^3}^2$ used in the definition of terms $J_{\mathbf{T}}(0, g)$ and $J_{\text{sc}}(g)$, respectively, are smooth, we see that these latter two maps are smooth.

Finally, we content ourselves with noticing that the asserted properties for the object function J_{in} are proven similarly as above, and so the proof is complete. \square

Remark 7.4 A. The term $g \rightarrow J_{\text{DV}}(0, g)$ is not convex in U_{ad} . This is due to the fact that the Heaviside function is not convex (or concave). Similarly the term $f \rightarrow J_{\text{DV}}(f, 0)$ is not convex in U'_{ad} .

B. If we used the term $\|D_0 - \mathcal{D}(f, g)\|_{L^p(\mathbf{T})}$ instead of $\|D_0 - \mathcal{D}(f, g)\|_{L^p(\mathbf{T})}^p$ and similarly for the other terms of the objective function(s), we would get in part (i) of the preceding theorem 7.3 a (globally) Lipschitz continuous terms of the object function when H is replaced with H_ϵ .

7.2.3. Computation of Initial Solutions. One possibility to help the optimization process is to compute the initial solution for actual (global) optimization method as accurately and rapidly as possible. We suggest the following approach for $p = 2$, and consider its details only in the case of the external radiotherapy. The computations for internal radiotherapy (formulated below) are analogous and thus omitted.

The spaces $W^2(G \times S \times I)$, $T^2(\Gamma)$ and $\tilde{W}^2(G \times S \times I)$ have Hilbert space structures, the inner products being respectively the following ones

$$\langle \psi, v \rangle_{W^2(G \times S \times I)} = \langle \psi, v \rangle_{L^2(G \times S \times I)} + \langle \omega \cdot \nabla \psi, \omega \cdot \nabla v \rangle_{L^2(G \times S \times I)}$$

$$\langle h, g \rangle_{T^2(\Gamma)} = \langle h, g \rangle_{L^2(\Gamma, |\omega \cdot \nu| d\sigma d\omega dE)}$$

and

$$\langle \psi, v \rangle_{\tilde{W}^2(G \times S \times I)} = \langle \psi, v \rangle_{W^2(G \times S \times I)} + \langle \gamma(\psi), \gamma(v) \rangle_{T^2(\Gamma)}.$$

In the product space $W^2(G \times S \times I)^3$ we use, as before, the inner product

$$\langle \psi, v \rangle_{W^2(G \times S \times I)^3} = \sum_{j=1}^3 \langle \psi_j, v_j \rangle_{W^2(G \times S \times I)},$$

where $\psi = (\psi_1, \psi_2, \psi_3)$, $v = (v_1, v_2, v_3) \in W^2(G \times S \times I)^3$, and similarly for other product spaces.

As is standard when $p = 2$, the formulas related to the optimal control system in the context of the transport equation are written below by using the relevant *variational equations* (based on the Green formula (8)). For example, the finite element method (FEM) schemes can be naturally implemented applying this formulation.

Let $f \in L^2(G \times S \times I)^3$ and $g \in T^2(\Gamma_-)^3$. Then $\psi \in \tilde{W}^2(G \times S \times I)^3$ is a solution of the problem

$$(192) \quad \begin{aligned} (-\mathbf{A} + \Sigma - K)\psi &= f, \\ \psi|_{\Gamma_-} &= g \end{aligned}$$

if and only if

$$(193) \quad B(\psi, v) = F(v), \quad \forall v \in \tilde{W}^2(G \times S \times I).$$

where $B(\cdot, \cdot)$ is a bilinear form given by

$$(194) \quad B(\psi, v) = -\langle \psi, \omega \cdot \nabla v \rangle_{L^2(G \times S \times I)^3} + \langle \psi, (\Sigma^* - K^*)v \rangle_{L^2(G \times S \times I)} \\ + \sum_{j=1}^3 \int_{\partial G \times S \times I} (\omega \cdot \nu)_+ \psi_j v_j d\sigma d\omega dE, \quad \text{for } \psi, v \in \tilde{W}^2(G \times S \times I)^3,$$

and where F is a linear form

$$(195) \quad F(v) = \langle f, v \rangle_{L^2(G \times S \times I)^3} + \sum_{j=1}^3 \int_{\partial G \times S \times I} (\omega \cdot \nu)_- g_j v_j d\sigma d\omega dE, \quad v \in \tilde{W}^2(G \times S \times I)^3$$

where $\Sigma^* = \Sigma$ and $K^* \psi^* = (K_1^* \psi^*, K_2^* \psi^*, K_3^* \psi^*)$ with

$$(K_j^* \psi^*)(x, \omega, E) = \sum_{k=1}^3 \int_{S \times I} \sigma_{jk}(x, \omega, \omega', E, E') \psi_k^*(x, \omega', E') d\omega' dE', \quad j = 1, 2, 3.$$

As above $(\omega \cdot \nu)_\pm$ are the positive and negative parts of $\omega \cdot \nu$, respectively. It is to be pointed out that the bilinear form B is not symmetric.

The existence result of the solution to the problem (192) in the variational form (when $p = 2$) corresponding to the Theorem 5.14 (where $p = 1$) is the following.

Theorem 7.5 Under the assumptions (67), (68), (69), (77), (78), for all $f \in L^2(G \times S \times I)^3$ and all $g \in T^2(\Gamma_-)^3$, there exists a unique $\psi \in \tilde{W}^2(G \times S \times I)^3$ such that (193) is holds.

Proof. The proof is an application of standard Hilbert space methods (e.g. using the Lions-Lax-Milgram theorem), and hence omitted here (see [51]).

Alternatively, one can adapt the proofs of Theorems 5.6 and 5.14 to the case $p = 2$, using the additional assumption (69), (78) made above. \square

We formulate the corresponding *adjoint problem* in the variational form. Define a bilinear form $B^*(\cdot, \cdot)$ by

$$(196) \quad B^*(\psi^*, v) = \langle \psi^*, \omega \cdot \nabla v \rangle_{L^2(G \times S \times I)^3} + \langle \psi^*, (\Sigma - K)v \rangle_{L^2(G \times S \times I)} \\ + \sum_{j=1}^3 \int_{\partial G \times S \times I} (\omega \cdot \nu)_- \psi_j^* v_j d\sigma d\omega dE \quad \text{for } \psi^*, v \in \tilde{W}^2(G \times S \times I)^3,$$

and, for a given $f^* \in L^2(G \times S \times I)^3$ and $g^* \in T^2(\Gamma_+)^3$, a linear form by

$$(197) \quad F^*(v) = \langle f^*, v \rangle_{L^2(G \times S \times I)^3} + \sum_{j=1}^3 \int_{\partial G \times S \times I} (\omega \cdot \nu)_+ g_j^* v_j d\sigma d\omega dE, \quad v \in \tilde{W}^2(G \times S \times I)^3.$$

For the adjoint problem, we have existence and uniqueness result similar to the above theorem.

Theorem 7.6 Assuming that (67), (68), (69), (77), (78) hold, then for every $f^* \in L^2(G \times S \times I)^3$ and $g^* \in T^2(\Gamma_+)^3$, there exists a unique $\psi^* \in \tilde{W}^2(G \times S \times I)^3$

such that

$$(198) \quad B^*(\psi^*, v) = F^*(v), \quad \forall v \in \tilde{W}^2(G \times S \times I).$$

Proof. We omit the proof, which is essentially based on Lions-Lax-Milgram Theorem (as the proof of Theorem 7.5); see [26], Lemma 4.4.4.1, p. 234. \square

The equation (198) is the variational form of the adjoint problem

$$(199) \quad (\mathbf{A}^* + \Sigma^* - K^*)\psi^* = f^*, \\ \psi^*|_{\Gamma_+} = g^*.$$

From the operator theoretical point of view, the above existence result for adjoint problem is based on the fact that for a densely defined closed operator $A : X \rightarrow X$ in Hilbert space X whose range $R(A^*)$ is closed in X , one has $R(A^*) = N(A)^\perp$ and $N(A^*) = R(A)^\perp$ (cf. [53], Section 2.8). In (199)

$$\mathbf{A}^*\psi^* = (\omega \cdot \nabla \psi_1^*, \omega \cdot \nabla \psi_2^*, \omega \cdot \nabla \psi_3^*), \quad \psi^* \in D(\mathbf{A}^*) := W^2(G \times S \times I)^3$$

where $\Sigma^* = \Sigma$ and K^* is as above. By the Green's formula (8) we see that

$$(200) \quad B(\psi, \psi^*) = B^*(\psi^*, \psi), \quad \text{for all } \psi, \psi^* \in \tilde{W}^2(G \times S \times I)$$

Recall that the flux to dose operator $D : L^2(G \times S \times I)^3 \rightarrow L^2(G)$ is

$$(D\psi)(x, \omega, E) = \sum_{j=1}^3 \int_{S \times I} \kappa_j(x, E) \psi_j(x, \omega, E) d\omega dE,$$

and that D is bounded. We find that its adjoint operator $D^* : L^2(G) \rightarrow L^2(G \times S \times I)^3$ is

$$(201) \quad D^*d = (\kappa_1, \kappa_2, \kappa_3)d, \quad \text{for } d \in L^2(G).$$

In external radiotherapy we have $\psi = \psi(0, g)$ and $\mathcal{D}(0, g) = D(\psi(0, g))$. We shall denote $\psi(g) = \psi(0, g)$ and $\mathcal{D}(g) = \mathcal{D}(0, g)$. Suppose that $d_{\mathbf{T}} \in L^2(\mathbf{T})$, $d_{\mathbf{C}} \in L^2(\mathbf{C})$, $d_{\mathbf{N}} \in L^2(\mathbf{N})$ are some given dose distributions (for example, they may be constants). We define an object function

$$(202) \quad J(g) = c_{\mathbf{T}} \|d_{\mathbf{T}} - \mathcal{D}(g)\|_{L^2(\mathbf{T})}^2 + c_{\mathbf{C}} \|d_{\mathbf{C}} - \mathcal{D}(g)\|_{L^2(\mathbf{C})}^2 \\ + c_{\mathbf{N}} \|d_{\mathbf{N}} - \mathcal{D}(g)\|_{L^2(\mathbf{N})}^2 + c \|g\|_{T^2(\Gamma_-)^3}^2,$$

with strictly positive constants $c_{\mathbf{T}}, c_{\mathbf{C}}, c_{\mathbf{N}}, c > 0$. In practice, only one type of particles are inflowing simultaneously (usually photons or electrons) but we can formulate a more general result which includes this more realistic situation. We denote (here the source $f = 0$)

$$F(v) = (Fg)(v) := \sum_{j=1}^3 \int_{\partial G \times S \times I} (\omega \cdot \nu)_- g_j v_j d\sigma d\omega dE = \langle g, \gamma_-(v) \rangle_{T^2(\Gamma_-)^3}$$

and, as before,

$$U_{\text{ad}} = \{g \in T^2(\Gamma_-)^3 \mid g \geq 0\}.$$

In what follows, we shall write $b_+ = \max\{0, b\}$ for the positive part of $b \in \mathbb{R}$, and $a_+ = ((a_1)_+, (a_2)_+, (a_3)_+)$ when $a = (a_1, a_2, a_3) \in \mathbb{R}^3$. We have the following optimality result.

Theorem 7.7 Suppose that the assumptions (67), (68), (77) and (78) are satisfied. Then the minimum $\min_{g \in U_{\text{ad}}} J(g)$ exists and is realized at the point $g = \bar{g}$ given by

$$(203) \quad \bar{g} = N(\gamma_-(\psi^*)) := \frac{1}{c}(\gamma_-(\psi^*))_+,$$

where the pair $(\psi, \psi^*) \in \tilde{W}^2(G \times S \times I)^3 \times \tilde{W}^2(G \times S \times I)^3$ is the unique solution of the coupled non-linear system of variational equations

$$(204) \quad \begin{aligned} B^*(\psi^*, v) + 2c_{\mathbf{T}} \langle D\psi, Dv \rangle_{L^2(\mathbf{T})} + 2c_{\mathbf{C}} \langle D\psi, Dv \rangle_{L^2(\mathbf{C})} + 2c_{\mathbf{N}} \langle D\psi, Dv \rangle_{L^2(\mathbf{N})} \\ = 2c_{\mathbf{T}} \langle d_{\mathbf{T}}, Dv \rangle_{L^2(\mathbf{T})} + 2c_{\mathbf{C}} \langle d_{\mathbf{C}}, Dv \rangle_{L^2(\mathbf{C})} + 2c_{\mathbf{N}} \langle d_{\mathbf{N}}, Dv \rangle_{L^2(\mathbf{N})} \\ B(\psi, v) = \langle N(\gamma_-(\psi^*)), \gamma_-(v) \rangle_{T^2(\Gamma_-)^3}, \end{aligned}$$

for all $v \in \tilde{W}^2(G \times S \times I)^3$.

Proof. By Lemma 7.2 the dose operator $\mathcal{D} : T^2(\Gamma_-)^3 \rightarrow L^2(G)$ is a bounded linear operator. Hence the object function $J : T^2(\Gamma_-)^3 \rightarrow \mathbb{R}$ is differentiable and strictly convex (see e.g. the proof of Theorem 7.3; note that the last term makes it strictly convex). Furthermore, J is bounded from below (in fact, it is non-negative), $U_{\text{ad}} \subset T^2(\Gamma_-)^3$ is convex and $\lim_{\|g\|_{T^2(\Gamma_-)^3} \rightarrow \infty, g \in U_{\text{ad}}} J(g) = \infty$. Therefore, there exists a unique minimum \bar{g} of J in U_{ad} and the necessary and sufficient conditions for the minimality of \bar{g} are (see e.g. [36])

$$(205) \quad J'(\bar{g})(\tilde{w} - \bar{g}) \geq 0, \quad \forall \tilde{w} \in U_{\text{ad}},$$

$$(206) \quad B(\psi(\bar{g}), v) = (F\bar{g})(v), \quad \forall v \in \tilde{W}^2(G \times S \times I)^3.$$

Let

$$(e_{\mathbf{T}}h)(x) = \begin{cases} h(x), & x \in \mathbf{T} \\ 0, & x \in G \setminus \mathbf{T} \end{cases}$$

for a function $h \in L^2(\mathbf{T})$ (the extension by zero onto G) and similarly we define extensions by zero for functions $h \in L^2(\mathbf{C})$ and $h \in L^2(\mathbf{N})$ onto G , respectively. The differential of $J'(g)$ is, recalling that $\mathcal{D}g = D(\psi(g)) =: D\psi(g)$,

$$(207) \quad \begin{aligned} J'(g)w = & 2c_{\mathbf{T}} \langle D\psi(g) - d_{\mathbf{T}}, D\psi(w) \rangle_{L^2(\mathbf{T})} + 2c_{\mathbf{C}} \langle D\psi(g) - d_{\mathbf{C}}, D\psi(w) \rangle_{L^2(\mathbf{C})} \\ & + 2c_{\mathbf{N}} \langle D\psi(g) - d_{\mathbf{N}}, D\psi(w) \rangle_{L^2(\mathbf{N})} + 2c \langle g, w \rangle_{T^2(\Gamma_-)^3} \\ = & 2c_{\mathbf{T}} \langle e_{\mathbf{T}}(D\psi(g) - d_{\mathbf{T}}), D\psi(w) \rangle_{L^2(G)} + 2c_{\mathbf{C}} \langle e_{\mathbf{C}}(D\psi(g) - d_{\mathbf{C}}), D\psi(w) \rangle_{L^2(G)} \\ & + 2c_{\mathbf{N}} \langle e_{\mathbf{N}}(D\psi(g) - d_{\mathbf{N}}), D\psi(w) \rangle_{L^2(G)} + 2c \langle g, w \rangle_{T^2(\Gamma_-)^3} \\ = & 2c_{\mathbf{T}} \langle D^*e_{\mathbf{T}}(D\psi(g) - d_{\mathbf{T}}), \psi(w) \rangle_{L^2(G)^3} + 2c_{\mathbf{C}} \langle D^*e_{\mathbf{C}}(D\psi(g) - d_{\mathbf{C}}), \psi(w) \rangle_{L^2(G)^3} \\ & + 2c_{\mathbf{N}} \langle D^*e_{\mathbf{N}}(D\psi(g) - d_{\mathbf{N}}), \psi(w) \rangle_{L^2(G)^3} + 2c \langle g, w \rangle_{T^2(\Gamma_-)^3}. \end{aligned}$$

Denoting

$$f^* := c_{\mathbf{T}}D^*e_{\mathbf{T}}(D\psi(g) - d_{\mathbf{T}}) + c_{\mathbf{C}}D^*e_{\mathbf{C}}(D\psi(g) - d_{\mathbf{C}}) + c_{\mathbf{N}}D^*e_{\mathbf{N}}(D\psi(g) - d_{\mathbf{N}}),$$

we have $f^* \in L^2(G \times S \times I)^3$, and so by Theorem 7.6 there exists a unique $\psi^* \in \tilde{W}^2(G \times S \times I)^3$ such that

$$(208) \quad B(v, \psi^*) = B^*(\psi^*, v) = -\langle f^*, v \rangle_{L^2(G \times S \times I)^3}, \quad \forall v \in \tilde{W}^2(G \times S \times I)^3.$$

Moreover, by definition $\psi(w) \in \tilde{W}^2(G \times S \times I)^3$, for any $w \in T^2(\Gamma_-)^3$, as the unique solution (by Theorem 7.5) of the problem (193) (with $g = w$ and $f = 0$), satisfies

$$(209) \quad B(\psi(w), v) = (Fw)(v), \quad \forall v \in \tilde{W}^2(G \times S \times I)^3.$$

Hence we have

$$(210) \quad \begin{aligned} 2 \langle f^*, \psi(w) \rangle_{L^2(G \times S \times I)^3} &= -2B(\psi(w), \psi^*) = -2(Fw)(\psi^*) \\ &= -2 \sum_{j=1}^3 \int_{\partial G \times S \times I} (\omega \cdot \nu)_- w_j \psi_j^* d\sigma d\omega dE \\ &= \langle -2\gamma_-(\psi^*), w \rangle_{T^2(\Gamma_-)^3}, \end{aligned}$$

where $\gamma_- : W^2(G \times S \times I) \rightarrow L^2_{\text{loc}}(\Gamma_-, |\omega \cdot \nu| d\sigma d\omega dE)$ as introduced in Section 2, but now in the context of L^p -spaces with $p = 2$, instead of $p = 1$, which was the case there. Combining the previous expressions (207) and (210) thus leads to

$$(211) \quad J'(g)w = 2 \langle f^*, \psi(w) \rangle_{L^2(G \times S \times I)^3} + 2c \langle g, w \rangle_{T^2(\Gamma_-)^3}$$

$$(212) \quad = \langle -2\gamma_-(\psi^*) + 2cg, w \rangle_{T^2(\Gamma_-)^3}.$$

Choosing for \tilde{w} in the condition (205) subsequently $w + \bar{g}$ and 0, we see that

$$(213) \quad J'(\bar{g})w \geq 0, \quad \forall w \in U_{\text{ad}}$$

$$(214) \quad J'(\bar{g})\bar{g} = 0.$$

Hence, by (211) and (213) one has

$$(215) \quad \langle -\gamma_-(\psi^*) + c\bar{g}, w \rangle_{T^2(\Gamma_-)^3} \geq 0, \quad \forall w \in U_{\text{ad}},$$

and so for each component $j = 1, 2, 3$,

$$(216) \quad -\gamma_-(\psi_j^*) + c\bar{g}_j \geq 0 \text{ a.e. in } \Gamma_-.$$

On the other hand, due to (214) we have

$$(217) \quad \langle -\gamma_-(\psi^*) + c\bar{g}, \bar{g} \rangle_{T^2(\Gamma_-)^3} = 0,$$

and so by (216) for each $j = 1, 2, 3$,

$$\bar{g}_j(-\gamma_-(\psi_j^*) + c\bar{g}_j) = 0 \text{ a.e. in } \Gamma_-.$$

From this, using again (216) and the fact that $\bar{g} \geq 0$, one concludes that

$$\bar{g}_j = \frac{1}{c} \max\{0, \gamma_-(\psi_j^*)\}, \quad j = 1, 2, 3,$$

which is the claim (203). Finally, substituting this into the equations (with $\psi = \psi(\bar{g})$),

$$\begin{aligned} B(\psi, v) &= (F\bar{g})(v), \\ B^*(\psi^*, v) &= -2 \langle f^*, v \rangle_{L^2(G \times S \times I)^3}, \end{aligned}$$

and noticing that

$$\begin{aligned} \langle f^*, v \rangle_{L^2(G \times S \times I)^3} &= c_{\mathbf{T}} \langle D\psi(g) - d_{\mathbf{T}}, Dv \rangle_{L^2(\mathbf{T})} + c_{\mathbf{C}} \langle D\psi(g) - d_{\mathbf{C}}, Dv \rangle_{L^2(\mathbf{C})} \\ &\quad + c_{\mathbf{N}} \langle D\psi(g) - d_{\mathbf{N}}, Dv \rangle_{L^2(\mathbf{N})}, \end{aligned}$$

we get the system of equations (204) for the pair (ψ, ψ^*) . This completes the proof. \square

Remark 7.8 If we choose the whole space $\tilde{U}_{\text{ad}} = T^2(\Gamma_-)^3$ as an admissible set instead of U_{ad} (i.e. if non-negativity of admissible controls was not imposed), we would find by considerations similar to those in the above proof that the following variation of Theorem 7.7 holds:

Under the assumptions (67), (68), (77) and (78), the minimum $\min_{g \in \tilde{U}_{\text{ad}}} J(g)$ exists and is realized at $g = \bar{g}$ given by

$$(218) \quad \bar{g} = \frac{1}{c} \gamma_-(\psi^*) =: N'(\gamma_-(\psi^*))$$

where the pair $(\psi, \psi^*) \in \tilde{W}^2(G \times S \times I)^3 \times \tilde{W}^2(G \times S \times I)^3$ is the solution of the coupled linear system of variational equations

$$(219) \quad \begin{aligned} B^*(\psi^*, v) + 2c_{\mathbf{T}} \langle D\psi, Dv \rangle_{L^2(\mathbf{T})} + 2c_{\mathbf{C}} \langle D\psi, Dv \rangle_{L^2(\mathbf{C})} + 2c_{\mathbf{N}} \langle D\psi, Dv \rangle_{L^2(\mathbf{N})} \\ = 2c_{\mathbf{T}} \langle d_{\mathbf{T}}, Dv \rangle_{L^2(\mathbf{T})} + 2c_{\mathbf{C}} \langle d_{\mathbf{C}}, Dv \rangle_{L^2(\mathbf{C})} + 2c_{\mathbf{N}} \langle d_{\mathbf{N}}, Dv \rangle_{L^2(\mathbf{N})} \\ B(\psi, v) = \langle N'(\gamma_-(\psi^*)), \gamma_-(v) \rangle_{T^2(\Gamma_-)^3}, \end{aligned}$$

which holds for all $v \in \tilde{W}^2(G \times S \times I)^3$.

By using this technique the initial solution for the full optimization problem of finding the minimum of J_{ex} on U_{ad} would be taken to be $\frac{1}{c}(\gamma_-(\psi_1^*))_+$. We point out that the equations (219) are linear, since $\psi^* \mapsto N'(\gamma_-(\psi^*))$ is linear, and therefore no iteration scheme is necessarily required in solving them. Presumably, however, the solution of non-linear optimization problem given in Theorem 7.7 should give a more accurate initial solution $N(\gamma_-(\psi^*))$ for the full optimization problem $\min_{g \in U_{\text{ad}}} J_{\text{ex}}(g)$, but this question will not be explored any further in this paper. Similar observation is concerning the internal therapy optimization described below.

In internal therapy $g = 0$ and so $\psi = \psi(f) := \psi(f, 0)$ and $\mathcal{D}(f) = D(\psi(f))$. The object function for the initial solution may be

$$(220) \quad \begin{aligned} J(f) = & c_{\mathbf{T}} \|d_{\mathbf{T}} - \mathcal{D}(f)\|_{L^2(+bfT)}^2 + c_{\mathbf{C}} \|d_{\mathbf{C}} - \mathcal{D}(f)\|_{L^2(\mathbf{C})}^2 \\ & + c_{\mathbf{N}} \|d_{\mathbf{N}} - \mathcal{D}(f)\|_{L^2(\mathbf{N})}^2 + c \|f\|_{L^2(G \times S \times I)^3}^2. \end{aligned}$$

and

$$U'_{\text{ad}} = \{f \in L^2(G \times S \times I)^3 \mid f \geq 0\}.$$

By arguments analogous to those used to prove Theorem 7.7 lead to the next result.

Theorem 7.9 Assume that (67), (68), (77), (78) hold. Then the minimum $\min_{f \in U'_{\text{ad}}} J(f)$ exists at the point $f = \bar{f} \in U'_{\text{ad}}$ where

$$(221) \quad \bar{f} = \frac{1}{c}(\psi^*)_+ =: N(\psi^*),$$

and the pair $(\psi, \psi^*) \in \tilde{W}_{-,0}^2(G \times S \times I)^3 \times \tilde{W}_{+,0}^2(G \times S \times I)^3$ is the solution of the coupled non-linear system of variational equations

$$(222) \quad \begin{aligned} B^*(\psi^*, v) + 2c_{\mathbf{T}} \langle D\psi, Dv \rangle_{L^2(\mathbf{T})} + 2c_{\mathbf{C}} \langle D\psi, Dv \rangle_{L^2(\mathbf{C})} + 2c_{\mathbf{N}} \langle D\psi, Dv \rangle_{L^2(\mathbf{N})} \\ = 2c_{\mathbf{T}} \langle d_{\mathbf{T}}, Dv \rangle_{L^2(\mathbf{T})} + 2c_{\mathbf{C}} \langle d_{\mathbf{C}}, Dv \rangle_{L^2(\mathbf{C})} + 2c_{\mathbf{N}} \langle d_{\mathbf{N}}, Dv \rangle_{L^2(\mathbf{N})} \\ B(\psi, v) = \langle N(\psi^*), v \rangle_{L^2(G \times S \times I)^3}, \end{aligned}$$

for all $v \in \tilde{W}^2(G \times S \times I)^3$.

Proof. We shall content ourselves here with sketching briefly the part of proof leading to (221), as this will be referred to in the remark that follows. Computations similar to those leading to (215) in the proof of Theorem 7.7, would give in the current context,

$$(223) \quad \langle -\psi^* + c\bar{f}, w \rangle_{L^2(G \times S \times I)^3} \geq 0, \quad \forall w \in U'_{\text{ad}},$$

hence

$$-\psi^* + c\bar{f} \geq 0 \text{ a.e. in } G \times S \times I,$$

and those leading to (217) would give

$$\langle -\psi^* + c\bar{f}, \bar{f} \rangle_{L^2(G \times S \times I)^3} = 0.$$

Since $\bar{f} \geq 0$ as $\bar{f} \in U'_{\text{ad}}$, we thus get

$$(224) \quad \bar{f}(-\psi^* + c\bar{f}) = 0 \text{ a.e. in } G \times S \times I,$$

from which (221) easily follows. \square

As we mentioned these solutions can be utilized as the initial solution for the (global) optimization but they are not ready solutions for the treatment planning.

Remark 7.10 Here we discuss some other choices of admissible sets. In [22] (see also [23]) one considers monoenergetic model for one species of particles. The existence and analogous optimal control formulas as above have been shown for the internal therapy when $f = f(x)$, that is when f is independent of the direction ω and energy E . This corresponds to the situation where one chooses for the admissible control the set (see below)

$$\tilde{U}'_{\text{ad}} = \{f \in L^2(G) \mid f \geq 0\}.$$

The practical availability for delivery is nowadays typically this kind of. Moreover, in the referred paper they considered a term of the objective function of the type $c \|f - f_0\|_{L^2(G)}^2$ instead of $c \|f\|_{L^2(G)}^2$, where $f_0 \in L^2(G)$ is a known source distribution.

Assume that $f_0 = 0$ (the generalization for $f_0 \neq 0$ is straightforward). Supposing, moreover, that admissible controls are independent of E , i.e. $f = f(x, \omega)$,

$$\tilde{U}'_{\text{ad}} = \{f \in L^2(G \times S) \mid f \geq 0\},$$

one gets the following necessary condition for optimal control $f = \bar{f}$:

$$(225) \quad \bar{f} = \frac{1}{c|I|} \left(\int_I \psi^* dE \right)_+ =: \tilde{N}(\psi^*)$$

and $(\psi, \psi^*) \in \tilde{W}_{-,0}^2(G \times S \times I)^3 \times \tilde{W}_{+,0}^2(G \times S \times I)^3$ is the solution of the coupled non-linear system of equations

$$(226) \quad \begin{aligned} B^*(\psi^*, v) + c_{\mathbf{T}} \langle D\psi, Dv \rangle_{L^2(\mathbf{T})} + c_{\mathbf{C}} \langle D\psi, Dv \rangle_{L^2(\mathbf{C})} + c_{\mathbf{N}} \langle D\psi, Dv \rangle_{L^2(\mathbf{N})} \\ = c_{\mathbf{T}} \langle d_{\mathbf{T}}, Dv \rangle_{L^2(\mathbf{T})} + c_{\mathbf{C}} \langle d_{\mathbf{C}}, Dv \rangle_{L^2(\mathbf{C})} + c_{\mathbf{N}} \langle d_{\mathbf{N}}, Dv \rangle_{L^2(\mathbf{N})} \\ B(\psi, v) = \left\langle \tilde{N}(\psi^*), v \right\rangle_{L^2(G \times S \times I)^3}, \end{aligned}$$

for all $v \in \tilde{W}^2(G \times S \times I)^3$. Above, $|I|$ denotes the length of the interval I .

That the optimal solution \bar{f} indeed has the above form (225) can be seen from the proof of Theorem 7.9, where (223) now holds for all $w \in \tilde{U}'_{\text{ad}}$, which gives

$-\int_I \psi^* dE + c|I|\bar{f} \geq 0$, and eventually the corresponding version of equation (224) would be

$$\bar{f}(-\int_I \psi^* dE + c|I|\bar{f}) = 0,$$

which leads directly to (225).

Finally, assuming that admissible controls f are independent of both E and ω , i.e. $f = f(x)$,

$$\tilde{U}'_{\text{ad}} = \{f \in L^2(G) \mid f \geq 0\},$$

one gets the following a necessary condition for optimal control $f = \bar{f}$:

$$(227) \quad \bar{f} = \frac{1}{4\pi c|I|} \left(\int_{S \times I} \psi^* dE d\omega \right)_+ =: \tilde{N}(\psi^*)$$

where $(\psi, \psi^*) \in \tilde{W}_{-,0}^2(G \times S \times I)^3 \times \tilde{W}_{+,0}^2(G \times S \times I)^3$ is the solution of the coupled non-linear system of variational equations

$$(228) \quad \begin{aligned} B^*(\psi^*, v) + c_{\mathbf{T}} \langle D\psi, Dv \rangle_{L^2(\mathbf{T})} + c_{\mathbf{C}} \langle D\psi, Dv \rangle_{L^2(\mathbf{C})} + c_{\mathbf{N}} \langle D\psi, Dv \rangle_{L^2(\mathbf{N})} \\ = c_{\mathbf{T}} \langle d_{\mathbf{T}}, Dv \rangle_{L^2(\mathbf{T})} + c_{\mathbf{C}} \langle d_{\mathbf{C}}, Dv \rangle_{L^2(\mathbf{C})} + c_{\mathbf{N}} \langle d_{\mathbf{N}}, Dv \rangle_{L^2(\mathbf{N})}, \\ B(\psi, v) = \left\langle \tilde{N}(\psi^*), v \right\rangle_{L^2(G \times S \times I)^3}, \end{aligned}$$

for all $v \in \tilde{W}^2(G \times S \times I)^3$. The arguments leading to (227) are easy adaptations to the set \tilde{U}'_{ad} of the steps between (223)-(224) in the proof of Theorem 7.9, precisely as discussed above when justifying (225).

A similar necessary formula can be obtained in the case of external therapy which can be seen from (217). When g is independent of energy E we have

$$(229) \quad \bar{g} = \frac{1}{c|I|} \left(\int_I \gamma_-(\psi^*) dE \right)_+ =: \tilde{N}(\gamma_-(\psi^*))$$

when $\psi^* \in$ is the solution of the coupled nonlinear system of variational equations

$$(230) \quad \begin{aligned} B^*(\psi^*, v) + c_{\mathbf{T}} \langle D\psi, Dv \rangle_{L^2(\mathbf{T})} + c_{\mathbf{C}} \langle D\psi, Dv \rangle_{L^2(\mathbf{C})} + c_{\mathbf{N}} \langle D\psi, Dv \rangle_{L^2(\mathbf{N})} \\ = c_{\mathbf{T}} \langle d_{\mathbf{T}}, Dv \rangle_{L^2(\mathbf{T})} + c_{\mathbf{C}} \langle d_{\mathbf{C}}, Dv \rangle_{L^2(\mathbf{C})} + c_{\mathbf{N}} \langle d_{\mathbf{N}}, Dv \rangle_{L^2(\mathbf{N})} \\ B(\psi, v) = (F(\tilde{N}(\gamma_-(\psi^*))) (v) \end{aligned}$$

for all $v \in \tilde{W}^2(G \times S \times I)^3$. In this case we have

$$U_{\text{ad}} = \{g \in L^2(\Gamma'_-), |\omega \cdot \nu| d\sigma d\omega)^3 \mid g \geq 0\}$$

where $\Gamma'_- = \{(y, \omega) \in \partial G \times S \mid \omega \cdot \nu(y) < 0\}$. The independence of g from angular ω is not reasonable in external therapy.

Finally, we notice that all the above formulas of optimal solutions can be applied in the case where only one species of particles is incoming or it is as a source in tissue (simply choose $g = (g_1, 0, 0)$ and so on).

Remark 7.11 Existence and formulas of optimal control for convex differentiable object functions on convex domains exists also for time-dependent (infinite dimensional) control systems (see e.g. [49], Chapter 7).

Remark 7.12 In the case where the actual object function J_{ex} in (188) or (189) is differentiable at a (local) optimal point $\bar{g} \in U_{\text{ad}}$ a necessary condition is that

$$(231) \quad J'_{\text{ex}}(\bar{g})(g - \bar{g}) \geq 0 \text{ for all } g \in U_{\text{ad}} \cap B(\bar{g}, r),$$

where $B(\bar{g}, r)$ is the open ball of radius $r > 0$ around \bar{g} in $T^2(\Gamma_-)^3$.

On the other hand, if the admissible set is taken to be the whole space $\tilde{U}_{\text{ad}} = T^1(\Gamma_-)^3$, the condition (231) reduces to

$$(232) \quad J'_{\text{ex}}(\bar{g}) = 0.$$

For globally convex object function the condition (232) is both necessary and sufficient for the global optimal control point $\bar{g} \in U_{\text{ad}}$ (when $J'_{\text{ex}}(\bar{g})$ exists). Similar facts are true for the object function J_{in} . Recall that if a convex function $U \rightarrow \mathbb{R}$ has a minimum, it is necessarily global minimum even if the function is not differentiable. This implies especially that when the dose volume constraint is not included in the object function, the (local) gradient based optimization methods can be applied "on the sets where gradient exists". For extensive literature of needed optimization and numerical analysis and techniques we refer to the recent monograph [3].

7.2.4. Proposed Optimization Strategy. The final optimization, that is, the inverse radiation treatment planning, could be realized in the following three phases:

1. Compute the initial solution by Theorem 7.7 or by its modification given in Remark 7.10. This step consists of carrying out *convex differentiable optimization*. However, it is not sufficient by itself because the optimal plan (control) obtained for the (partial) object function (202) may produce unwanted dose to the critical organ/normal tissue.

2. Compute the optimal plan for object function (188) *without* the dose volume constraint (i.e. $c_{\text{CV}} = 0$), using as the initial guess the solution obtained in step 1. This step involves carrying out *Lipschitz continuous convex optimization*.

3. Compute the optimal plan for the object function (188) *with* the dose volume constraint (i.e. $c_{\text{CV}} > 0$), using as the initial guess the solution acquired in step 2. In this step one needs to perform *non-convex optimization*, and needs, therefore, a global optimization scheme.

One may optionally add between the steps 2. and 3. an intermediate optimization phase where the object function for the dose volume constraint is replaced by a Lipschitz continuous term

$$J_{\text{DV},\epsilon}(0, g) = \left(\left(v_C - \frac{1}{\mathcal{L}^3(\mathbf{C})} \int_{\mathbf{C}} H_{\epsilon}(\mathcal{D}(0, g)(x) - d_C) dx \right)_- \right)^p,$$

where H_{ϵ} is a continuous approximation of the Heaviside function H , for example

$$(233) \quad H_{\epsilon}(x) = \begin{cases} 0, & x \leq 0 \\ \frac{1}{\epsilon}x, & 0 \leq x \leq \epsilon \\ 1, & x \geq \epsilon \end{cases}.$$

Alternatively, this modified (smooth) dose volume term could be used in step 3. When $p = 2$ the further modified term

$$\tilde{J}_{\text{DV},\epsilon}(0, g) = \left(v_C - \frac{1}{\mathcal{L}^3(\mathbf{C})} \int_{\mathbf{C}} H_{\epsilon}(\mathcal{D}(0, g)(x) - d_C) dx \right)^2$$

turns out to be differentiable and (globally) Lipschitz continuous, which might be used to facilitate the optimization. It should be pointed out, however, that the inherent *non-convexity* of J_{DV} cannot be removed.

7.2.5. *Some Remarks on the Discrete Problem and Modelling.* In practical radiation treatment planning the coupled Boltzmann transport equation must be discretized. Commonly used methods for discretization are finite element method (FEM), or collocation method in the spatial variable x and in the energy variable E and spherical harmonics in the angle variable ω (cf. e.g. [1], [6], [9]). We do not consider these issues here but list some of the challenges that the resulting discrete problems involve. We shall denote below the set of $n \times m$ matrices by $M(n \times m)$.

1) Applying appropriate discretization methods the finite dimensional approximation of the transport equation (176) is of the form

$$(234) \quad A\alpha = B\beta$$

where $A \in M(3N \times 3N)$ and $B \in M(3N \times 3M)$. The approximative components of the solution ψ of (176) are

$$\psi_j \approx \tilde{\psi}_j = \tilde{\psi}_j(f, g) := \sum_{k=1}^N \alpha_{jk} \phi_k(x, \omega, E), =: \Psi_j(x, \omega, E) \alpha \quad j = 1, 2, 3,$$

where $\{\phi_k \mid k = 1, \dots, N\}$ is a basis for a chosen finite dimensional subspace W_N of $\tilde{W}^2(G \times S \times I)^3$ (in the case $p = 2$), and the coefficients α_{jk} are obtained from $\alpha = A^{-1}B\beta$ (we omit here the detailed arrangements of matrices, for details see e.g. [9]). Above $\Psi_j(x, \omega, E) \in M(1 \times N)$ is a matrix, which is computed with the help of basis functions.

For example, each element ϕ_k of the above basis might be taken to be finite linear combinations of (tensor) products of the form $\varphi_p(x)\Omega_q(\omega)\mathcal{E}_r(E)$, with $\varphi_p \in H^1(G)$ (the standard Sobolev space for $p = 2$), $\Omega_q \in L^2(S)$ and $\mathcal{E}_r \in L^2(I)$.

The column vector $\beta \in \mathbb{R}^M$ contains (is calculated from) the discretized known input data (internal sources and/or incoming flux). For example, in the case of external radiotherapy we put

$$(235) \quad g_j \approx \sum_{k=1}^M \beta_{jk} \eta_k(y, \omega, E)$$

where η_k is an appropriate basis of M -dimensional subspace of $T^2(\Gamma_-)$. We see that

$$(236) \quad g_j \approx \mathcal{G}_j(y, \omega, E) \beta$$

where $\mathcal{G}_j(y, \omega, E) \in M(1 \times M)$ (computed with the help of basis functions η_k). Note that using the above matrices

$$(237) \quad \psi \approx \Psi(x, \omega, E) \alpha$$

and

$$(238) \quad g \approx \mathcal{G}(y, \omega, E) \beta$$

for some matrices $\Psi(x, \omega, E) \in M(1 \times (3N))$ and $\mathcal{G}(y, \omega, E) \in M(1 \times (3M))$ (obtained with the help of matrices $\Psi_j(x, \omega, E)$ and $\mathcal{G}_j(y, \omega, E)$, respectively).

In the case where FEM scheme is applied, the matrices A and B can be computed in a standard way from the variational form of the transport equations. The conditions (77) and (78) guarantee the *convergence* of the FEM scheme by the well-known Cea's estimate (for $p = 2$) since they imply the boundedness and coercitivity of the bilinear form $B(., .)$ given in section 7.2.3 in appropriate Hilbert spaces.

By the above the dose operator D is approximated by

$$D(x) \approx \tilde{D}(f, g)(x) := \tilde{D}(x) = \sum_{j=1}^3 \sum_{k=1}^N \int_S \int_I \alpha_{jk} \kappa_j(x, E) \phi_k(x, \omega, E) d\omega dE, =: \mathcal{D}(x)\alpha$$

for some $\mathcal{D}(x) \in M(1 \times (3N))$, while the terms for the approximative object function, e.g. in the case of external radiotherapy, are given (for general $p > 1$) by

$$\begin{aligned} J_{\mathbf{T}}(0, g) &\approx \|D_0 - \mathcal{D}(\cdot)\alpha\|_{L^p(\mathbf{T})}^p =: J_{\mathbf{T}}(\alpha) \\ J_{\mathbf{C}}(0, g) &\approx \left\| (D_C - \mathcal{D}(\cdot)\alpha)_- \right\|_{L^p(\mathbf{C})}^p =: J_{\mathbf{C}}(\alpha) \\ J_{\mathbf{N}}(0, g) &\approx \left\| (D_N - \mathcal{D}(\cdot)\alpha)_- \right\|_{L^p(\mathbf{N})}^p =: J_{\mathbf{N}}(\alpha) \\ J_{\text{DV}}(0, g) &\approx \left(\left(v_C - \frac{1}{\mathcal{L}^3(\mathbf{C})} \int_{\mathbf{C}} H((\mathcal{D}(\cdot))(x) - d_C) dx \right)_- \right)^p =: J_{DC}(\alpha) \\ J_{\text{sc}}(0, g) &\approx \|\Psi(\cdot, \cdot, \cdot)\alpha\|_{L^p(G \times S \times I)^3}^p =: J_{\text{sc}}(\alpha) \end{aligned}$$

and so the approximation of the whole object function is

$$(239) \quad J = J(\alpha) = J_{\mathbf{T}}(\alpha) + J_{\mathbf{C}}(\alpha) + J_{\mathbf{N}}(\alpha) + J_{\text{DV}}(\alpha) + J_{\text{sc}}(\alpha).$$

Substituting $\alpha = A^{-1}B\beta$ to (239) we get the object function with the help of control variables β .

The dimensionality of the discretized problem (234) is typically very large in the number N of unknowns α_{jk} , although it can be reduced by techniques like the adaptation of the grid. This is one of the main drawbacks of the method because to form the inverse A^{-1} one must calculate the inverse of the very large dimensional matrix, even if matrices involved in FEM, as is well known, are sparse. Iterative algorithms must be applied in solving the equation $A\alpha = B\beta$. One can partially avoid this problem by applying the so-called parametrization, described below (cf. [9], [52]), but then another difficulty arises in constructing the parametrization operator (based e.g. on the Singular Value Decomposition (SVD)).

The initial solution for the discrete problem can be calculated as follows. Denote

$$(240) \quad D(\psi, v) := 2c_{\mathbf{T}} \langle D\psi, Dv \rangle_{L^2(\mathbf{T})} + 2c_{\mathbf{C}} \langle D\psi, Dv \rangle_{L^2(\mathbf{C})} + 2c_{\mathbf{N}} \langle D\psi, Dv \rangle_{L^2(\mathbf{N})}$$

and

$$(241) \quad d(v) := 2c_{\mathbf{T}} \langle d_{\mathbf{T}}, Dv \rangle_{L^2(\mathbf{T})} + 2c_{\mathbf{C}} \langle d_{\mathbf{C}}, Dv \rangle_{L^2(\mathbf{C})} + 2c_{\mathbf{N}} \langle d_{\mathbf{N}}, Dv \rangle_{L^2(\mathbf{N})}.$$

Then the variational equations (203)-(204) are

$$(242) \quad \begin{aligned} B^*(\psi^*, v) + D(\psi, v) &= d(v) \\ B(\psi, v) &= \frac{1}{c} \langle (\gamma_-(\psi^*))_+, \gamma_-(v) \rangle_{L^2(\Gamma_-)^3}, \quad v \in \tilde{W}^2(G \times S \times I)^3. \end{aligned}$$

The discrete approximation of the system (242) is of the form

$$(243) \quad \begin{aligned} A^*\xi + \mathbf{D}\alpha &= \mathbf{d} \\ A\alpha &= \mathbf{g}(\xi) \end{aligned}$$

where $\mathbf{D} \in M(3N \times 3N)$, $\mathbf{d} \in M(3N \times 1)$, \mathbf{g} is a piecewise linear (non)function and

$$(244) \quad \psi_j^* \approx \tilde{\psi}_j^* := \sum_{k=1}^N \xi_{jk} \phi_k.$$

The optimal control is approximately

$$(245) \quad \bar{g} = \frac{1}{c}(\gamma_-(\psi^*))_+ \approx \frac{1}{c}(\gamma_-(\tilde{\psi}^*))_+$$

where $\tilde{\psi}^* := (\tilde{\psi}_1^*, \tilde{\psi}_2^*, \tilde{\psi}_3^*)$ is obtained from (244) with the help of ξ .

2) The term *parametrization* above means the following concept. The discrete system (234) can be written as

$$(246) \quad (A \quad -B) \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0,$$

where $(A \quad -B) \in M(N \times (N + M))$ and $\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \in M((N + M) \times 1)$. Let $P \in M((N + M) \times N')$ be a matrix such that (246) holds if and only if

$$(247) \quad \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = P\tau$$

that is, $P \in M(N' \times 1)$ is the "basis generating matrix (operator) of the kernel $N((A \quad -B))$ ". Such a matrix P always exists and is called the *parametrization (operator/matrix)* of the system (234).

We observe that if Q is a matrix such that

$$(248) \quad (A \quad -B) Q (A \quad -B) = (A \quad -B)$$

then $P := I - Q (A \quad -B)$ is a parametrization. Especially, (248) is valid if $Q = (A \quad -B)^+$ is the Moore-Penrose pseudo-inverse of $(A \quad -B)$. Note that when applying (248) the dimension (number of rows and columns) of P is $N + M$ but it can be essentially reduced by omitting insignificant elements.

In virtue of (247) we have $\alpha = P_1\tau$, $\beta = P_2\tau$ for some matrices P_j , $j = 1, 2$ obtained from blocks of P . The object function becomes with the help of parameters τ as

$$(249) \quad J = J(\alpha) = J(P_1\tau) =: J(\tau).$$

The optimization problem becomes the following: Find the global minimum

$$(250) \quad \inf_{\tau \in U_{\text{ad}}^d} J(\tau)$$

where

$$(251) \quad U_{\text{ad}}^d := \{\tau \in \mathbb{R}^{N'} \mid g \approx \mathcal{G}(y, \omega, E)\beta = \mathcal{G}(y, \omega, E)P_2\tau \geq 0\}.$$

In the case where the basis $\{\eta_k\}$ is build up of positive step functions (zero-order splines), the interiors of supports of which are disjoint, we have $U_{\text{ad}}^d = \{\tau \in \mathbb{R}^{N'} \mid \beta = P_2\tau \geq 0\}$. Using higher order splines would, however, be preferred. An alternative possibility for taking care of the positivity of the approximative controls g is to add a penalty term of the form $c_{\text{ad}} \|(\mathcal{G}(\cdot, \cdot, \cdot)P_2\tau)_-\|_{T^2(\Gamma_-)}^p$ to the object function. No explicit inversion of the matrix A is needed. The essential problem in this approach is in constructing the parametrization P , approximatively, and preferably such that N' (the number of parameters) is small. Moreover, the algorithms used in this construction should be a iterative schemes, during which the accuracy can be controlled. Elements of P which are small enough should be neglected, such that the dimensionality of P gets decreased and its sparsity gets increased. Preliminary simulations have shown that this approach works at least in spatially 2D-situations

(cf. [9], where $N + M \approx 5000$, $N' \approx 100$). For applying the explained parametrization method, an initial solution τ for the optimization can be obtained e.g. as in [9], p. 110 (we omit the details here).

3) Another possibility to avoid inversions of huge matrices would be to utilize in computations the formulas given in Remark 5.19, that is to compute $\psi = \psi(f, g)$ from

$$(252) \quad \psi = \sum_{k=0}^{\infty} ((-\mathbf{A}_0 + \Sigma)^{-1} K)^k ((-\mathbf{A}_0 + \Sigma)^{-1} (f - (\Sigma - K)(Lg))) + Lg,$$

where $(-\mathbf{A}_0 + \Sigma)^{-1}$ can be explicitly obtained from (123). Alternatively, one could compute $\psi = \psi(f, g)$ approximately from (see (127))

$$(253) \quad \psi \approx \int_0^T \left[T(t/n_0) e^{-(t/n_0)\Sigma(x, \omega, E)} \sum_{k=0}^{N_0} \frac{1}{k!} ((t/n_0)K)^k \right]^{n_0} (f - (\Sigma - K)(Lg)) dt + Lg.$$

Substituting one of these expressions into

$$(\mathcal{D}(f, g))(x) = \sum_{j=1}^3 \int_{S \times I} \kappa_j(x, E) (\psi_j(f, g))(x, \omega, E) d\omega dE$$

one acquires the (approximate) dose as a function of f and g . Consequently, the object function $J = J(f, g)$ can be directly calculated from (185), (186), (187).

The initial solution \bar{g} (e.g. for external radio therapy) for applying this computational scheme is calculated from

$$\bar{g} = \frac{1}{c} (\gamma_-(\psi^*))_+,$$

where ψ^* is solved from the coupled system (see the proof of Theorem 7.7)

$$(254) \quad \begin{aligned} & (-\mathbf{A}^* + \Sigma^* - K^*)\psi^* + c_{\mathbf{T}} D^* e_{\mathbf{T}} D \psi + c_{\mathbf{C}} D^* e_{\mathbf{C}} D \psi + c_{\mathbf{N}} D^* e_{\mathbf{N}} D \psi \\ & \quad = c_{\mathbf{T}} D^* e_{\mathbf{T}} d_{\mathbf{T}} + c_{\mathbf{C}} D^* e_{\mathbf{C}} d_{\mathbf{C}} + c_{\mathbf{N}} D^* e_{\mathbf{N}} d_{\mathbf{N}}, \\ & (-\mathbf{A} + \Sigma - K)\psi = 0 \\ & \psi_{|\Gamma_+}^* = 0, \\ & \psi_{|\Gamma_-} = \frac{1}{c} (\gamma_-(\psi^*))_+, \end{aligned}$$

where the system of equations is equivalent to

$$(255) \quad \begin{pmatrix} -\mathbf{A}^* + \Sigma^* - K^* & c_{\mathbf{T}} D^* e_{\mathbf{T}} D + c_{\mathbf{C}} D^* e_{\mathbf{C}} D + c_{\mathbf{N}} D^* e_{\mathbf{N}} D \\ 0 & -\mathbf{A} + \Sigma - K \end{pmatrix} \begin{pmatrix} \psi^* \\ \psi \end{pmatrix} = \begin{pmatrix} c_{\mathbf{T}} D^* e_{\mathbf{T}} d_{\mathbf{T}} + c_{\mathbf{C}} D^* e_{\mathbf{C}} d_{\mathbf{C}} + c_{\mathbf{N}} D^* e_{\mathbf{N}} d_{\mathbf{N}} \\ 0 \end{pmatrix}$$

As far as the authors are aware of, computationally effective and stable techniques for solving (254) (for instance using formulas similar to (252), (253)) require further study.

4) Because of their strongly forward-peaked migration, it would be reasonable to use the Continuous Slowing Down Approximation (see the introduction) in the transport of electrons and positrons. When the solution of the transport equation is smooth enough (see section 6.1), higher order spline basis functions (along with related more rapid convergence results) could be used in numerical techniques like FEM.

5) Except for J_{DV} (see, however, the discussion at the end of Section 7.2.4), the terms of the discretized object function are (locally) Lipschitz continuous. Nonetheless, while they are convex, the terms J_T , J_C , J_N , J_{ad} , J_{sc} are not differentiable in general, except for the case $p = 2$ in which case J_T and J_{sc} are differentiable (see Theorem 7.3). The term J_{DV} , however, is non-convex, and therefore a global optimization strategy is needed if this constraint is to be taken into account in the treatment planning. There exist several global optimization algorithms well suited for Lipschitz continuous (not necessarily differentiable) object functions (e.g. [43]). Large dimensionality of the related (discretized) object function's variables is, however, a limiting factor for the application of these methods in practice.

6) Multicriteria optimization and related (interactive) decision making can be applied to the treatment planning applying the presented optimization schemes ([46]). In addition, we remark that optimization can be used simultaneously for external and internal therapy (which is not likely applied in practise).

7) As we mentioned in the introduction, in the case of external radiotherapy the incoming flux (or fluence) g can be essentially expressed using *beam parameters*, which is to be understood include relevant (controllable) variables like the energy of the incoming beam, multileaf collimator (MLC) leaf positions, the jaw positions as well as rotational parameters related to the gantry and collimator rotations etc. (this is by no means intended to be an exhaustive list). The dose optimization problem can then be put in the form where the object function is expressed in terms of beam parameters.

This approach has the advantage that device constraints can be taken into account at an early stage of the treatment planning. The main disadvantage, however, is that the resulting object function is likely to be highly *multiextremal*, and so effective global optimization algorithms are fundamental for the success of such an approach. Notice that the approach given here enables to optimize besides of position, the energies and angles of incoming flux(es) since $g = g(y, \omega, E)$.

8) Stochastic aspects (arising e.g. from delivery processes or patient motions during the treatment) can be taken into account by using as the transport model the so-called *stochastic Boltzmann transport equation*. Matters like inverse treatment planning interpreted as an optimal control (boundary) problem, existence of optimal control and its computation, exact controllability and so on, can be then considered in the (more general) framework of the stochastic calculus. For a glimpse of some recent advances in the context of stochastic BTE and its controllability, we refer e.g. to [38] and the references therein. Issues of exact controllability (and observability) are considered there for time-dependent monokinetic single particle transport equation.

9) We emphasize that in the computations of the object function, with the exception of the additional terms J_{sc} and J_{ad} , one only needs to know of the dose distribution

$$D(x) = \sum_{j=1}^3 \int_S \int_I \kappa_j(x, \omega) \psi_j(x, \omega, E) d\omega dE$$

which is a kind of a moment. It might thus be possible to develop iterative approximative methods for calculating the dose without explicitly solving ψ . These techniques lead to recursive computations of some tensors, which also seem to have a physical meaning.

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